DIGITAL SIMULATION AND OPTIMIZATION OF CATALYTIC REFORMING UNITS

A Thesis Submitted
In Partial Fulfilment of the Requirements
for the Degree of
MASTER OF TECHNOLOGY

By
ASHOK KUMAR SHARMA

to the

DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY KANPUR
MAY 1973
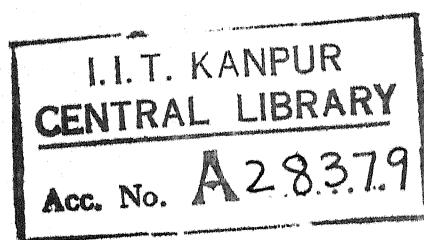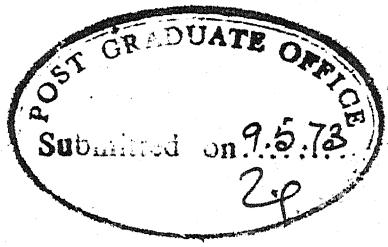
CERTIFICATE

This is to certify that the present work
'Digital Simulation and Optimization of Catalytic-
Reforming Units' has been carried out under my super-
vision and that this work has not been submitted
elsewhere for a degree.

(M. Gopala Rao)
Associate Professor
Department of Chemical Engg.
Indian Institute of Technology
Kanpur-208016, India

May 8, 1973

ACKNOWLEDGEMENTS

ABSTRACT

A mathematical model for the simulation of catalytic-reforming units has been developed. The model takes into account most of the complex reactions occuring in the process. The model was used to simulate on a digital computer two industrial Platforming units. Agreement between simulation results and plant data is very satisfactory. It has been found that the performance of an industrial unit can be improved significantly by changing some of the present operating conditions. An optimization routine to minimize the weight of catalyst and the operating cost has been developed. Further work can be done to combine mathematical models of inter heater and a flash unit with the present simulation model.

ABSTRACT

A mathematical model for the simulation of catalytic-reforming units has been developed. The model takes into account most of the complex reactions occuring in the process. The model was used to simulate on a digital computer two industrial Platforming units. Agreement between simulation results and plant data is very satisfactory. It has been found that the performance of an industrial unit ean be improved significantly by changing some of the present operating conditions. An optimization routine to minimize the weight of catalyst and the operating cost has been developed. Further work can be done to combine mathematical models of inter heater and a flash unit with the present simulation model.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

NOMENCLATURE

A	:	Aromatics produced, moles/mole of naphtha
C_p	:	Specific heat of the reaction mixture, Btu/(Degree Rankine.mole of feed to the first reactor)
d_p	:	Diameter of catalyst particle
d_t	:	Diameter of reactor
F_P	:	Pounds of feed to first reactor
F_T	:	Pound mole of feed to first reactor
g_c	:	Force-mass conversion factor
H	:	Hydrogen produced, moles/mole of naphtha
HC	:	Hydrocracked products produced, moles/mole of naphtha
L	:	Length of reactor
M_w	:	lb Molecular weight of feed to first reactor
MW_F	:	lb Molecular weight of naphtha
N	:	Number of reactors in series
N_{Re}	:	Reynold's number
P	:	Pressure, atm.
P_A	:	Partial pressure of aromatics, atm.
P_H	:	Partial pressure of hydrogen, atm.
P_N	:	Partial pressure of naphthenes, atm.
P_P	:	Partial pressure of paraffins, atm.
P_T	:	Total pressure, atm.
R	:	Gas constant
T	:	Temperature, $^{\circ}R$

T_i : Temperature of inlet stream to reactor i.

w : Weight of catalyst, lb.

W_i : Weight of catalyst in reactor i, lb.

X_{i5} : Temperature in reactor i.

X_{ij} : Extent of conversion for reaction (2.j) in reactor i, mole/mole of feed to first reactor of the series

XA : Mole fraction of aromatics in naphtha

XAI : Mole fraction of aromatics in feed to first reactor

XHCI : Mole fraction of C_5 and lower hydrocarbons in feed to first reactor

XHI : Mole fraction of hydrogen in feed to first reactor

XN : Mole fraction of naphthenes in naphtha

XNI : Mole fraction of naphthenes in feed to first reactor

XP : Mole fraction of paraffins in naphtha

XPI : Mole fraction of paraffins in feed to first reactor

ε : Porosity of catalyst bed

ϵ : Objective function

ρ_c : Density of catalyst bed, lb/ft^3

CHAPTER I

INTRODUCTION

Use of analogy and simulation has contributed a lot to progress of science and technology. Through analogy with familiar and simple events one can understand more complex phenomena of the world in which one lives. To test analogical conclusions, experiments have to be conducted which simulate the natural conditions one wishes to understand. Because of its very definition, an analogy or simulation can not be identical with realities of nature it attempts to represent.

As technology expands, the demand for laboratory simulation also expands. In some experiments, the parameters which govern the behaviour of the system under study are complex enough to restrain the experimenter from such a work. As a result modern research and technology have found digital and analog simulation not only expedient but also indispensable. And now with the advent of big and fast computers, one can manipulate the mathematical equations of the system, called mathematical model, with a reasonable degree of effort and cost.

Digital simulation is also of vital importance for the chemical industry as it can be used:

1. To facilitate design and operation of process or its parts.

2. To choose operating conditions for changed production pattern or increased production in an existing plant.

3. To study the effect of extreme ranges of operating conditions, some of which might be impractical or impossible to use in a pilot plant.

4. To compress or expand real time.

5. To compare various proposed designs and processes not yet in operation.

6. To test the hypothesis about a system or process before making a decision.

7. To study the effect of changes in variables and parameters with reproducible results.

8. To gain sufficient knowledge about the system to facilitate computer control.

It might appear from the discussion presented above that it is much better to analyse the system by digital-simulation than to analyse it by carrying out laboratory experiments or by pilot-plant studies. Unfortunately, there are certain limitations to the simulation technique as the accuracy of the results obtained by it depends largely on correctness of the mathematical model developed and the accuracy of the physical and chemical data that go into the model.

In India to meet the increasing demand of aromatics
(installed capacity of benzene in India has increased from
15,000 tons per annum in 1963 to 87,000 in 1969/70 and the
requirements for 1973/74 have been estimated at 1,40,000 tons)
a catalytic-reforming plant is being commissioned in Gujrat
State. At present the process know-how for this process which
uses naphtha as feed stock, is imported from the Western
European countries. Catalytic-reforming when combined with
solvent extraction or extractive distillation produces ,
benzene for ultimate conversion to phenol or styrene, toluene
for nitration purpose, xylene for plastics etc., in quanti-
ties far beyond the capacity of any other source to provide
these materials. Catalytic - reforming which goes under
various names such as Platforming (Universal Oil Product Co.),
Power-forming (Esso Research and Engineering Co.), Ultra-
forming (Oil Co. of Indiana), etc. is also used to upgrade
the octane number of straight run gasolines, naphtha and
other feed stocks. The hydrogen which is liberated in this
process can be ploughed back into heavier portion of crude
oil either by direct hydrocracking of heavy oil or by milder
hydrogenation to produce superior Diesel fuel or improved
charge stock to the catalytic cracking units. In order to
achieve self-sufficiency (partially or fully) in this important
process, it has been intended in the present work to simulate
the reactors system coming up in Gujrat State using the IBM
7044 computer.

Catalytic reforming is a high pressure and high temperature process which uses halogenated alumina coated with platinum as catalyst. Generally, three to five steel reactors packed with catalyst with an inter-heater before each are used in series. The reactor vessels are insulated by monolithic ceramic liners. Light gases which have about 85 percent hydrogen are seperated in flash unit from catalytic reformate. A part of this gas is used as recycle gas. Detailed process flow diagram is given in Fig. 1.

In the present study, a mathematical model has been developed to predict the product stream of a catalytic-reforming reactor system for a given feed composition, catalyst distribution, inlet temperature, inlet pressure and recycle ratio. The effects of temperature, pressure and recycle ratio have been studied. This mathematical model together with principles of calculus of variation, are used to write an algorithm to extremize an objective function with constraints on final product stream. Using this algorithm, respective objective functions involving total weight of catalyst, and operating costs have been minimized for a three, four, and five reactors set-up.

Present study deals only with the steady state behaviour of the process, dynamic response has not been studied. The composition of recycle gas from the flash unit
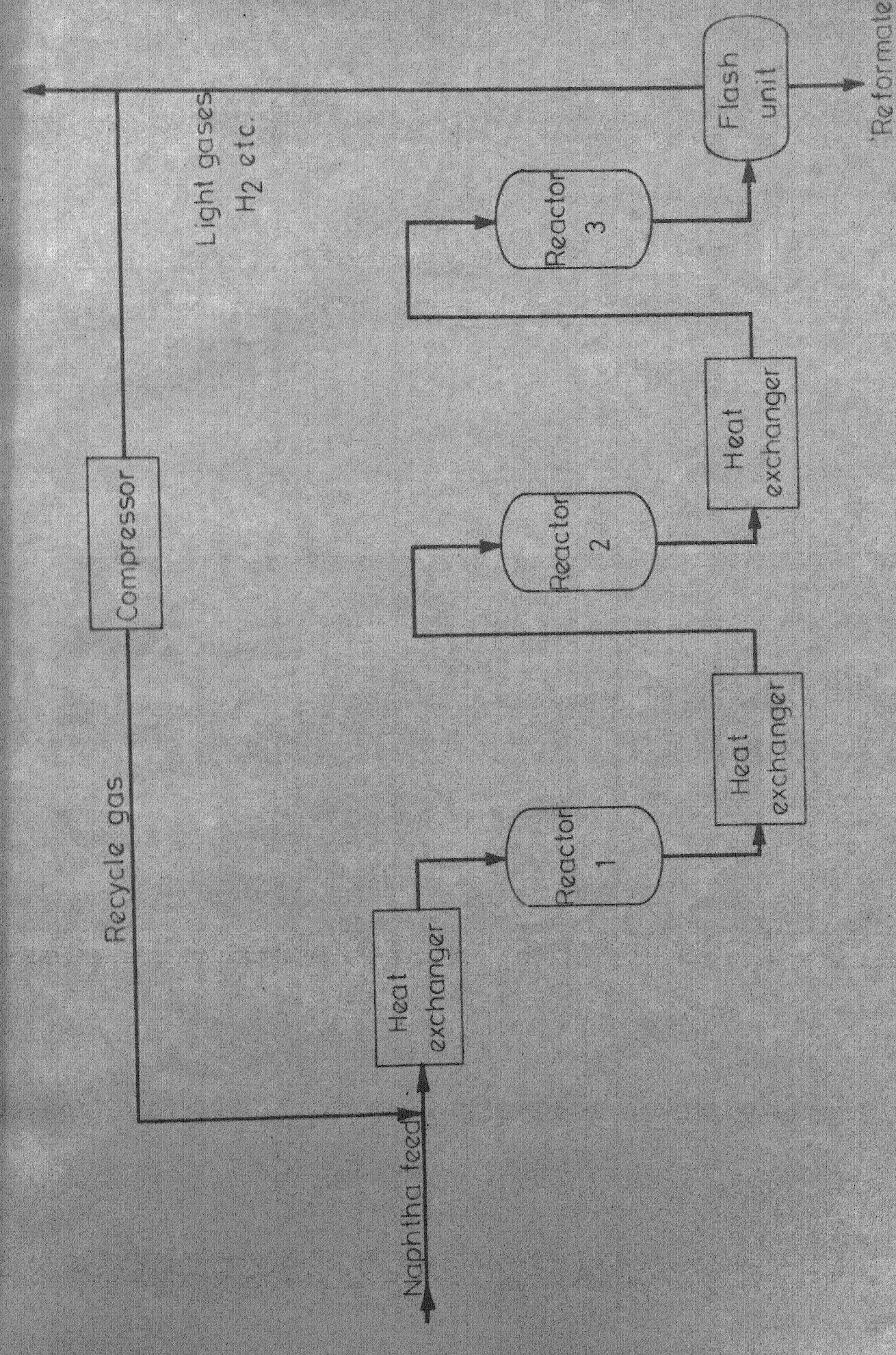
Fig 1 – Catalytic – Reforming Flow Diagram.

is not calculated, and instead a fixed composition is assumed. The effect of temperature, pressure and impurities in naphtha on the catalyst life is not considered.

CHAPTER II

LITERATURE ON CATALYTIC REFORMING REACTION

Many chemical reactions, some simple and some complex, constitute catalytic-reforming but the reactions leading to the formation of aromatics from naphthenes and paraffins are of greater importance. Under the catalytic-reforming conditions, dehydrogenation of naphthenic hydrocarbons is very rapid and contributes substantially for the yield of aromatics. These reactions are highly endothermic and result in somewhat to volumetric shrinkage since the aromatics product is denser than the parent naphthenes (1). Aromatics are also formed from naphthenic intermediate resulting from cyclization of paraffins. But this reaction is not obtained in most ideal sequences because even at a moderate severity level, naphthene dehydrogenation is close to completion while paraffin dehydrocyclization is still in the initial stages. Furthermore for all types of catalyst used commercially, the dehydrocyclization of paraffins is less efficient than dehydrogenation of naphthenes. For this reason, naphthene dehydrogenation to aromatics is considered to be the backbone of catalytic-reforming (2). Hydrocracking which is opposite of dehydrogenation from the stand point of yield and the heat of reaction, is also an important reaction. In this reaction high-molecular weight hydrocarbons decompose to lower-molecular-weight hydrocarbons.

As discussed above, catalytic-reforming is simultaneous dehydrogenation, cyclization and hydrocracking. One can imagine the complexity and cumbersomeness if rate expressions written for each carbon number compounds in the naphtha undergoing the reforming reactions, are to be solved. Kinetic studies have been done by taking each hydrocarbon seperately. Attempts have also been made to simplify the problem by treating naphtha to be of some average carbon number depending on its composition. In such studies Smith (3) has come out with a reaction model and rate equations which are reported to be applicable for naphtha feed stocks under widely used operating conditions for catalytic-reforming. Katrush and others (4) report that these kinetic equations fail to predict plant behaviour for Russian naphthas. For each reaction, the rate equations of each reaction used by Katrush et al, for three reactors in series have different rate constants for each reactor. Their results are based on the hypothesis that in the first reactor the main reaction is dehydrogenation,in the second dehydrogenation and cyclization, and in third dehydrocyclization, isomerization and hydrocracking. Recently Heningsen and Nielson (5) have came out with different reaction model and kinetic rate expressions. But these have been reported only for C_8 system and reactions occuring at $500^{\circ}C$ and 30 atm. The rate expression of Marianme Vermorner and others (6) who carried out their work seperately

are approximately the same as obtained by Smith. Smith (3) has proposed the following reaction model:

1. Naphthenes $\rightleftharpoons$ Aromatics + Hydrogen

$$C_n H_{2n} \rightleftharpoons C_n H_{2n-6} + 3H_2 \qquad (2.1)$$

2. Naphthenes + Hydrogen $\rightleftharpoons$ Paraffins

$$C_n H_{2n} + H_2 \rightleftharpoons C_n H_{2n+2} \qquad (2.2)$$

3. Paraffins + Hydrogen $\rightarrow$ Hydrocarbons

$$C_n H_{2n+2} + \frac{n-3}{2} H_2 \rightarrow \frac{n}{15} (CH_4 + C_2H_6 + \ldots C_5H_{12}) \qquad (2.3)$$

4. Naphthenes + Hydrogen $\rightarrow$ Hydrocarbons

$$C_n H_{2n} + \frac{n}{3} \rightarrow \frac{n}{15} (CH_4 + C_2H_6 + \ldots C_5H_{12}) \qquad (2.4)$$
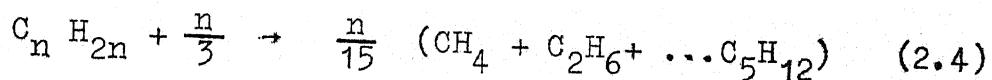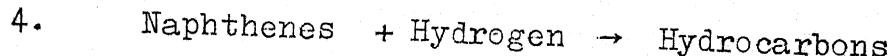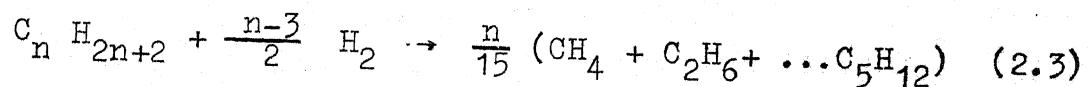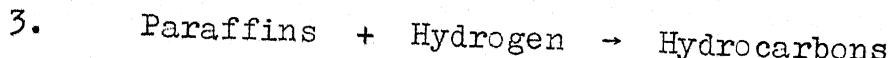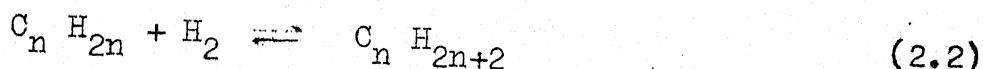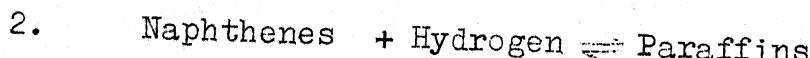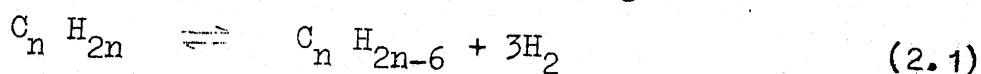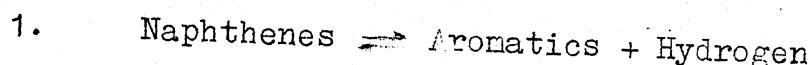
In the above reaction model, it has been assumed that the hydrocracking of aromatics is too slow and can be neglected. The stoichiometry of reaction (2.3)and(2.4)which shows that equal number of moles of methane, ethane, propane, butane and pentane are formed from hydrocracking of naphthenes and paraffins, has been derived from experimental observations, that these species are formed approximately in equal molar proportion.

From thermodynamical considerations, one expects catalytic reforming reactions to proceed at low pressures and high temperatures. But at high temperatures, coke gets deposited on the catalyst due to hydrocracking, which reduces the catalyst activity. Coke deposition can be overcome by

having a high hydrogen partial pressure which can be obtained
at higher operating pressures. It also reduces sulfur deposi-
tion on the catalyst by converting sulfur to hydrogen sulfide (7).
Operation at high pressures lengthens the time between regene-
rations, increases yield of aromatics and reduces the amount
of light end products by suppressing hydrocracking. But as the
pressure is increased beyond a certain limit, the yield of
aromatics deteriorates because of more hydrogenation of naphthe-
nes to paraffins.

Hydrogen partial pressure can also be increased by increas-
ing the hydrogen to hydrocarbon ratio which is direct function
of the recycle ratio.   Though at low recycle ratio more hydro-
gen can be formed, the partial pressure of hydrogen is not
sufficient to suppress the coke deposition on the catalyst.
Increase of hydrogen concentration can also reduce the yield
of aromatics because it reverses the order of desirable reac-
tions.

CHAPTER III

MATHEMATICAL MODELING AND SIMULATION

Assuming that hydrocracking of aromatics to hydrocarbons is negligible and methane, ethane, propane, butane and pentane are formed in equal molar proportions from the hydrocracking of naphthenes and paraffins, one can write the over all reaction model for catalytic - reforming reactions:

1.   Naphthenes $\rightleftharpoons$ Aromatics + Hydrogen
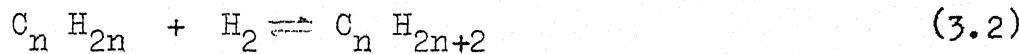
$$C_n H_{2n} \rightarrow C_n H_{2n-6} + 3H_2 \tag{3.1}$$

2.   Naphthenes + Hydrogen $\rightleftharpoons$ Paraffins

$$C_n H_{2n} + H_2 \rightleftharpoons C_n H_{2n+2} \tag{3.2}$$

3.   Paraffins + Hydrogen $\rightarrow$ Hydrocarbons

$$C_n H_{2n+2} + \frac{n-3}{3} H_2 \rightarrow \frac{n}{15} (CH_4 + C_2 H_6 + \ldots C_5 H_{12}) \tag{3.3}$$

4.   Naphthenes + Hydrogen $\rightarrow$ Hydrocarbons

$$C_n H_{2n} + \frac{n}{3} \rightarrow \frac{n}{15} (CH_4 + C_2 H_6 + \ldots C_5 H_{12}) \tag{3.4}$$
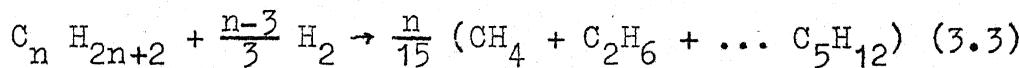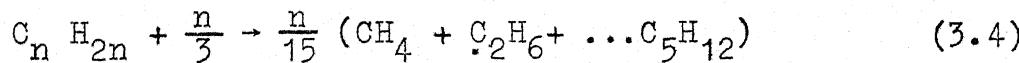
Furthermore, it has been found reasonable to assume that each of the three hydrocarbon classes eg. paraffins, naphthenes and aromatics in naphtha, has on the whole the same number of carbon atoms 'n'. Based on this, value of n can be obtained, by expressing molecular weight of naphtha in terms of molecular formula as shown below:

$$XP \ (C_n \ H_{2n+2}) + XN \cdot (C_n \ H_{2n}) + XA \ (C_n \ H_{2n-6}) = MW_F$$
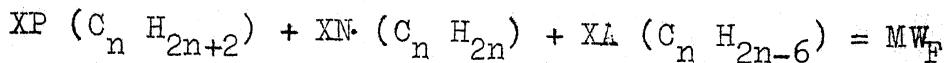
or $\quad n = \dfrac{1}{14} \ (MW_F - 2 \ XP + 6 \ XA)$

Experimental data shows that heats of reactions are nearly independent of component molecular weight over the range normally encountered in reforming process, when based on moles of H_2 entering into the reaction. Based on this, kinetic rate expressions and heat of reaction for reactions (2.1) through (2.4) as reported by Smith (3) are given below:

1. $\quad r_1 = k_1 \ (P_N - \dfrac{P_A \ P_H^3}{K_1})$

<u>lb mole of naphthenes converted to aromatics</u>
hr (lb of catalyst)

(3.5)

$k_1 = \exp \ (23.21 - 34750/T) \quad \dfrac{\text{lb mole naphthenes}}{\text{hr (lb cat) atm}}$

$K_1 = \exp \ (46.15 - 46045/T) \quad atm^3$

$\Delta H_1 = 30500 \quad \dfrac{Btu}{16 \ \text{mole} \ H_2 \ \text{produced}}$

2. $\quad r_2 = k_2 \ (P_N \ P_H - \dfrac{P_P}{K_2})$

<u>lb mole of naphthenes converted to paraffins</u>
(hr. lb cat.)

(3.6)

$k_2 = \exp \ (35.98 - 59600/T) \quad \dfrac{\text{lb mole naphthenes}}{\text{hr. lb cat atm}^2}$

$K_2 = \exp \ (8000/T - 7.12) \quad atm^{-1}$

$\Delta H_2 = -19000 \quad \dfrac{Btu}{16 \ \text{mole} \ H_2 \ \text{consumed}}$

3. $r_3 = k_3 \dfrac{P_P}{P_T}$ (3.7)

$k_3 = \exp(42.97 - 62300/T) \dfrac{\text{lb mole paraffins}}{\text{hr (lb. cat)}}$

$\Delta H_3 = -24300 \dfrac{\text{Btu}}{\text{mole } H_2 \text{ consumed}}$

4. $r_4 = k_4 \dfrac{P_N}{P_T}$ (3.8)

$k_4 = \exp(42.97 - 62300/T) \dfrac{\text{lb mole naphthenes}}{\text{hr. (lb cat)}}$

$\Delta H_4 = -22300 \dfrac{\text{Btu}}{\text{mole } H_2 \text{ consumed}}$

Under catalytic- reforming conditions for which tempe-
rature and pressure are of the order of 800-1000°F and 15-50
atmospheres respectively, the reaction system is always in
gaseous state. Preliminary calculations showed that the
flow of these gases in the reactors is in highly turbulent
region with N_{Re} of the order of 15,000 or more. Since there
is sufficient packing on both the sides of reactors, it can
be assumed that the flow of gases is in fully developed tur-
bulent flow region in the catalyst zone. Catalytic-reform-
ing reactors also have $L/d_p \gg 20$ and $d_t/d_p > 10$. For such
flow conditions and reactors one can safely assume a plug-flow
pattern (8).

If X_{i1}, X_{i2}, X_{i3} and X_{i4} are extents of reactions (2.1),
(2.2), (2.3) and (2.4); per mole of total feed F_T at a place in
reactor i, then the partial pressure terms appearing in the
rate equations can be written as follows:

$$P_A = P_T \quad \text{mole fraction of aromatics}$$

$$= P_T \quad \frac{\text{moles of aromatics}}{\text{Total moles}}$$

$$= P_T \quad \frac{XAI + X_{i1}}{1+3X_{i1}-X_{i2}+(\frac{n}{15}\cdot 5-1-\frac{n-3}{3})X_{i3}+(\frac{n}{15}\cdot 5-1-\frac{n}{3})X_{i4}}$$

$$= P_T \quad \frac{XAI + X_{i1}}{1+3X_{i1}-X_{i2}-X_{i4}}$$

$$P_N = P_T \quad \frac{XNI - (X_{i1}+X_{i2}+X_{i4})}{1+3X_{i1}-X_{i2}-X_{i4}}$$

$$P_P = P_T \quad \frac{XPI + X_{i2} - X_{i3}}{1+3X_{i1} - X_{i2} - X_{i4}}$$

$$P_H = P_T \quad \frac{XHI + 3X_{i1}-X_{i2}- \frac{n-3}{3} X_{i3} - \frac{n}{3} X_{i4}}{1+3X_{i1} - X_{i2} - X_{i4}}$$

Material balance for reaction (2.1) for a differential reactor section of catalyst weight Δw, gives:

$$\Delta X_{i1} \cdot F_T = r_1 \Delta w$$

or

$$\frac{dX_{i1}}{dw} = \frac{r_1}{F_T}$$

$$= k_1 \left(P_T \frac{(XNI -(X_{i1} + X_{i2} + X_{i4}))}{1+3X_{i1} - X_{i2} - X_{i4}} - \right.$$

$$\left. \frac{P_T^4 (XAI+X_{i1})(XHI+3X_{i1}-X_{i2}- \frac{n-3}{3}X_{i3}-\frac{n}{3}X_{i4})^3}{K_1(1+3X_{i1} - X_{i2} - X_{i4})^4} \right)/F_T$$

$$(3.9)$$

For reactions (2.2), (2.3) and (2.4) also similar relations are obtained:

$$\frac{dX_{i2}}{dw} = k_2 \left(\frac{P_T^2 (XNI - X_{i1} - X_{i2} - X_{i4})(XHI + 3X_{i1} - X_{i2} - \frac{n-3}{3} X_{i3} - \frac{n}{3} X_{i4})}{(1 + 3X_{i1} - X_{i2} - X_{i4})^2} \right.$$

$$\left. - \frac{P_T (XPI + X_{i2} - X_{i3})}{K_2 (1 + 3X_{i1} - X_{i2} - X_{i4})} \right) / F_T \qquad (3.10)$$

$$\frac{dX_{i3}}{dw} = k_3 \frac{(XPI + X_{i2} - X_{i3})}{(1 + 3X_{i1} - X_{i2} - X_{i4}) \cdot F_T} \qquad (3.11)$$

$$\frac{dX_{i4}}{dw} = k_4 \frac{(XNI - X_{i1} - X_{i2} - X_{i4})}{(1 + 3X_{i1} - X_{i2} - X_{i4}) F_T} \qquad (3.12)$$

Since reactions are carried out in an adiabatic reactor system, energy balance equation can be written as:

$$C_p \cdot F_T \cdot \Delta T = (\Delta X_{i1} \cdot 3(-\Delta H_1) + \Delta X_{i2}(-\Delta H_1)$$

$$+ \Delta X_{i3} \frac{n-3}{3} (-\Delta H_3) + \Delta X_{i4} \frac{n}{3} (-\Delta H_4)) \cdot F_T$$

Dividing both sides of the above equation by Δw, rearranging, and taking the limit $\Delta w \to 0$, one gets,

$$\frac{dT}{dw} = (3 \frac{dX_{i1}}{dw} (-\Delta H_1) + \frac{dX_{i2}}{dw} (-\Delta H_2) +$$

$$+ \frac{dX_{i3}}{dw} \frac{n-3}{3} (-\Delta H_3) + \frac{dX_{i4}}{dw} \frac{n}{3} (-\Delta H_4)) / C_p \qquad (3.13)$$

After manipulating the equation normally used for packed beds (9), pressure drop in the differential element can be written as follows:

$$\frac{dP}{dw} = \frac{(150(1-\epsilon)+1.75)(1-\epsilon).F_p^2.R.T.(1+3X_{i1}-X_{i2}-X_{i4})}{\rho_c.Area^3.d_p.g_c.\epsilon^3.M_w.P_T} \quad (3.14)$$

Initial and boundary conditions for reactor system are:

$$X_{1j}(0) = 0 \qquad j = 1,2,3,4 \qquad\qquad (3.15)$$

$$X_{ij}(0) = X_{i-1,j}(W_{i-1}) \qquad j = 1,2,3,4 \qquad (3.16)$$
$$i = 2,3,\ldots,N$$

Equation (3.9) through (3.14) together with (3.15) and (3.16) constitute the mathematical model for the reactor system.

SIMULATION:

Since fresh feed is mixed with the recycle gas before it is fed to the reactors, the solution of equations (3.9) through (3.14) can not be obtained without knowing the recycle gas composition. Calculations for recycle gas composition are difficult because of two reasons:

Firstly adequate equilibrium data to calculate the composition of the gas seperated from product stream of the last reactor in the flash unit are not available.

Secondly some iterative scheme has to be used because of the recycle stream.

The problem can be simplified by assuming recycle gas composition to be the one, normally encountered in catalytic reforming plants. This is justified because of the following reasons:

1. Recycle gas has about 85 percent hydrogen on molar basis.

2. Major portion of the hydrocarbons in the recycle gas is constituted by C_5 and lower hydrocarbons, which do not take part in the reaction model assumed for the present study.

Preliminary calculations also show that a small change in the recycle gas composition does not cause any appreciable effect on the product stream from the reactors.

Specific heat, C_p, occuring in equation (3.13) cannot be treated as constant because the reactions are carried out under adiabatic conditions, and temperature changes are large. Specific heats can be assumed to be linear functions of temperature and it has been found from preliminary calculations that any improvement in this regard does not improve results of simulation to any appreciable extent.

In the specific heat calculations, it was assumed that the carbon-number component break-up of naphthenes, paraffins (higher than C_6) and aromatics in the reaction mixture is the same as it is in the feed to the first reactor. This

assumption was made necessary due to lack of information on the composition (in terms of carbon numbers) of naphthenes, paraffins and aromatics in the product streams. For simplicity, they are lumped together as three species, paraffins, naphthenes and aromatics.

If specific heats of aromatics, naphthenes, paraffins, hydrogen, hydrocarbons coming in feed and hydrocarbons produced by hydrocracking can be represented by the following linear functions of temperature, (details of which appear in Appendix C);

$$C_{pA} = FA(1) + FA(2).T$$

$$C_{pN} = FN(1) + FN(2).T$$

$$C_{pP} = FP(1) + FP(2).T$$

$$C_{pH} = FH(1) + FH(2).T$$

$$C_{pHC} = FHC(1) + FHC(2).T$$

$$C_{pHCI} = FHCI(1) + FHCI(2).T \ ;$$

the specific heat, C_p, of reaction mixture can be written as,

$$C_p = (XAI + X_{i1}) \ C_{pA} + (XNI - X_{i1} - X_{i2} - X_{i4}) \ C_{pN}$$

$$+ (XPI + X_{i2} - X_{i3}) \ C_{pP}$$

$$+ (XHI + 3X_{i1} - X_{i2} - \frac{n-3}{3} X_{i3} - \frac{n}{3} X_{i4}) \ C_{pH}$$

$$+ (\frac{n}{3} X_{i3} + \frac{n}{3} X_{i4}) \ C_{pHC} + XHCI. \ C_{pHCI}$$

or $\quad C_p = \displaystyle\sum_{j=1}^{2} \big[XAI.FA(j)+XPI.FP(j)+XNI.FN(j)$

$\qquad + XHI.FH(j)+XHCI.FHCI(j)$

$\qquad + (FA(j)-FN(j)+3.FH(j))\ X_{i1}$

$\qquad + (FP(j)-FN(j)-FH(j))\ X_{i2}$

$\qquad + (FHC(j).\frac{n}{3} - FP(j)-FH(j).\frac{n-3}{3})\ X_{i3}$

$\qquad + (FHC(j)\ \frac{n}{3} - FN(j) - FH(j)\ \frac{n}{3})\ X_{i4}\ ](T)^{j-1}$

Pressure drops along the reactors and inter-heaters
in catalytic-reforming plants are of the order of .7 to 1.7
atmospheres. These are small in comparison to the operating
pressures. Preliminary calculations show that the results
of simulation obtained by assuming the pressure as invariant
are approximately the same as those obtained by considering
the pressure-drop along length of the reactor. Based on this,
equation (3.14) was dropped from the system model i.e. dp/dw
has been put equal to zero.

Using the recycle gas composition given in Appendix A,
the system equations (3.9) through (3.13) together with (3.15)
and (3.16) were solved on the IBM 7044 digital computer by
using the fourth-order Runge-Kutta method.

CHAPTER IV

OPTIMIZATION

OBJECTIVE:

Since throughput for a catalytic reforming plant is generally very large, even a small shift in the operating conditions and various parameters of the reactor system from optimum values can change the economic pattern of the process. Reactor sizes, weight of the catalyst, heat exchanger duties and compressor size constitute major share of fixed capital investment, while catalyst life, heat duty and power in-puts to the compressor, determine major part of the operating costs. The variables, temperatures of inlet streams, recycle ratio, operating pressure and number of reactors determine both fixed and operating costs. Higher temperature of the inlet stream though giving rise to higher catalytic activity initially, increases hydrocracking which in turn decreases catalyst activity because of the coke deposition on the catalyst. This can be overcome by having high hydrogen partial pressure which is determined by the choice of the operating pressure and the recycle ratio.

The choice of the operating variables can be subjected to various objectives such as minimization of operating cost or weight of the catalyst for a fixed throughput and fixed

quality of product, or for maximization of venture profit
when installing a new plant. Generally constraints on the
product are there to ensure certain production rate of
aromatics and a certain concentration of these in the
reformate. There are also constraints on the lowest and
the heighest values of temperature which are determined
by reaction rate considerations and catalyst life.

Mathematically, ε, the objective function can be func-
tion of catalyst weight, catalyst distribution in different
reactors, catalyst life, furnace sizes and duties and com-
pressor size and duty.

The constraints are the following:

$$g_1(X_{N1}, X_{N2}, X_{N3}, X_{N4}) = C_1$$

$$g_2(X_{N1}, X_{N2}, X_{N3}, X_{N4}) = C_2$$

$$1260 \leq T_i \leq 1460$$

In the present study, minimization of catalyst weight
and minimization of operating cost are the two objective
functions seperately investigated. Catalyst life is a
variable, which is difficult to take into account. For
example the operational life of catalyst depends on tempe-
rature, pressure, recycle ratio, and feed composition. Very
little data are available in literature. In the present
study it is assumed that catalyst is replaced after every
10.8 months. Also, effect of pressure and recycle ratio
was not considered in optimization routine.

MATHEMATICAL DEVELOPMENT:

The system under study has reactors in series. Each reactor is represented by five differential equations and is related to the reactor next in the series by four equations. Extremization of an objective function ϵ , for such a system which has constraints also on the final product stream can be done by using Calculus of Variation and Pontryagin principle of optimality (10,11,12,13,14,15).

If W_i is weight of catalyst in reactor i, the reactor system can be described by the following equations:

$$\frac{dX_{ij}}{dW} = f_{ij}$$

or
$$\dot{X}_{ij} = f_{ij} \tag{4.1}$$

X_{ij} corresponds to extent of reaction(2,j)in reactor
i for j = 1,2,3,4 and

X_{i5} corresponds to temperature in reactor i.

The initial and boundary conditions for (4.1) are,

$$X_{1j}(0) = 0 \qquad j = 1,2,\ldots 4 , \tag{4.2}$$

since reactors are in series

$$X_{i,j}(W_i) = X_{i+1,j}(0) \qquad j = 1,2,3,4 \tag{4.3}$$
$$i = 1,2,\ldots N-1$$

Because of small changes in decision variables the _variational equations of the system_ can be constructed as,

$$\delta \dot{X}_{ij} = \sum_{k=1}^{5} \frac{\partial f_{ij}}{\partial X_{ik}} \delta X_{ik} + \text{higher order terms} \quad (4.4)$$

Similarly, variation in the objective function, which may depend on the weight of catalyst and various other parameters of the inlet and outlet stream at each reactor can be written as,

$$\delta \varepsilon = \sum_{l=1}^{N} \sum_{k=1}^{5} \left(\frac{\partial \varepsilon}{\partial X_{1k}(0)} \delta X_{1k}(0) + \frac{\partial \varepsilon}{\partial X_{1k}(W_1)} \delta X_{1k}(W_1) \right)$$

$$+ \sum_{l=1}^{N} \frac{\partial \varepsilon}{\partial W_1} \delta W_1 + \text{higher order terms} \quad (4.5)$$

Similarly, variations in the values of constraints, which depend on the outlet stream from the last reactor are,

$$\delta g_1 = \sum_{k=1}^{4} \frac{\partial g_1}{\partial X_{Nk}} \delta X_{Nk}(W_N) + \text{higher order terms} \quad (4.6)$$

$$\delta g_2 = \sum_{k=1}^{4} \frac{\partial g_2}{\partial X_{Nk}} \delta X_{Nk}(W_N) + \text{higher order terms} \quad (4.7)$$

In the further development, higher order terms have been neglected for the sake of simplicity.

It is readily seen that equations (4.2) and (4.3) for (4.4) become,

$$\delta X_{1j}(0) = 0 \qquad j = 1,2,3,4 \quad (4.8)$$

$$\delta X_{i,j}(W_i) = \delta X_{i+1,j}(0) \quad i = 1,2,\ldots,N-1 \quad (4.9)$$

Now multiply Equation (4.4) by arbitrary continuous functions $\lambda_{ij}(w)$ and integrate for $w = 0$ to $w = W_i + \delta W_i$. Thus,

$$\int_0^{W_i + \delta W_i} \lambda_{ij} \delta \dot{X}_{ij} \, dw = \int_0^{W_i + \delta W_i} \sum_{k=1}^{5} \frac{\partial f_{ij}}{\partial X_{ik}} \delta X_{ik} \lambda_{ij} \, dw \quad (4.10)$$

Integrating left hand side of eqn. (4.10) by parts,

$$\int_0^{W_i + \delta W_i} \lambda_{ij} \delta \dot{X}_{ij} \, dw = \lambda_{ij} \delta X_{ij} \Big|_0^{W_i + \delta W_i} - \int_0^{W_i + \delta W_i} \dot{\lambda}_{ij} \delta X_{ij} \, dw$$

$$(4.11)$$

$$\lambda_{ij} \delta X_{ij} \Big|_0^{W_i + \delta W_i} = \lambda_{ij}(W_i + \delta W_i) \delta X_{ij}(W_i + \delta W_i)$$

$$- \lambda_{ij}(0) \delta X_{ij}(0)$$

$$= \left[\lambda_{ij}(W_i) + \frac{\partial \lambda_{ij}(W_i)}{\partial w} \delta W_i \right] \cdot$$

$$\left[\delta X_{ij}(W_i) + \frac{\partial X_{ij}(W_i)}{\partial w} \delta W_i \right]$$

$$- \lambda_{ij}(0) \delta X_{ij}(0)$$

$$= \lambda_{ij}(W_i) \delta X_{ij}(W_i) + \lambda_{ij}(W_i) \cdot$$

$$f_{ij}(W_i) \delta W_i + \dot{\lambda}_{ij}(W_i) \delta W_i \delta X_{ij}(W_i)$$

$$+ \dot{\lambda}_{ij}(W_i) f_{ij}(W_i) \delta W_i \delta W_i$$

$$- \lambda_{ij}(0) \delta X_{ij}(0) \quad (4.12)$$

Neglecting second order terms in (4.12) and making use of (4.11), one gets from equation (4.10)

$$\lambda_{ij}(W_i) \, \delta X_{ij}(W_i) + \lambda_{ij}(W_i) \, f_{ij}(W_i) \, \delta W_i - \lambda_{ij}(0) \, \delta X_{ij}(0)$$

$$= \int_0^{W_i + \delta W_i} \sum_{k=1}^{5} \frac{\partial f_{ij}}{\partial X_{ik}} \, \delta X_{ik} \, \lambda_{ij} \, dw + \int_0^{W_i + \delta W_i}$$

$$\dot{\lambda}_{ij} \, \delta X_{ij} \, dw \qquad (4.13)$$

Now add following to equation (4.5):

1. Equation (4.13) for i = 1,2,...N and j = 1,2,...5

2. Multiplications of right hand side of equations (4.6) and (4.7) by arbitrary constants η_1 and η_2.

3. Multiplications of equation (4.9) with ν_{ij} for i = 1,2,..., N-1 and j = 1,2,3,4.

If ε_1 and ε_2 have fixed values C_1 and C_2 respectively i.e., $\delta \varepsilon_1 = \delta \varepsilon_2 = 0$.

$$\delta \varepsilon = \sum_{l=1}^{N} \left(\frac{\partial \varepsilon}{\partial W_l} + \sum_{k=1}^{5} \lambda_{lk}(W_l) \, f_{lk}(W_l) \right) \delta W_l$$

$$+ \sum_{l=1}^{N-1} \sum_{k=1}^{4} \left(\lambda_{lk}(W_l) + \nu_{lk} + \frac{\partial \varepsilon}{\partial X_{lk}} \right) \delta X_{lk}(W_l)$$

$$+ \sum_{k=1}^{5} (\lambda_{Nk}(W_N) + n_1 \frac{\partial g_1}{\delta X_{Nk}(W_N)} + n_2 \frac{\partial g_2}{\delta X_{Nk}(W_N)}$$

$$+ \frac{\partial \epsilon}{\delta X_{Nk}(W_N)}) \delta X_{Nk}(W_N) - \sum_{l=1}^{N-1} (\lambda_{l5}(W_l) + \frac{\partial \epsilon}{\delta X_{l5}(W_l)}) \cdot$$

$$\delta X_{l5}(W_l) - \sum_{l=2}^{N-1} \sum_{k=1}^{4} (\lambda_{lk}(0) + \nu_{l-1,k} - \frac{\partial \epsilon}{\partial X_{lk}}) \cdot$$

$$\delta X_{lk}(0) - \sum_{l=1}^{N} (\lambda_{l5}(0) - \frac{\partial \epsilon}{\partial X_{l5}(0)}) \delta X_{l5}(0)$$

$$- \sum_{k=1}^{4} (\lambda_{1k}(0) \delta X_{1k}(0) - \frac{\partial \epsilon}{\partial X_{1k}(0)}) \delta X_{1k}(0)$$

$$- \sum_{l=1}^{N} \sum_{k=1}^{5} \int_{0}^{W_l + \delta W_l} (\dot{\lambda}_{lk} + \sum_{m=1}^{5} \lambda_{im} \frac{\partial f_{lm}}{\partial X_{lk}}) \delta X_{1k} \cdot dw \quad (4.14)$$

There are certain terms which are not at one's disposal, namely, $\delta X_{1k}(W_1)$ in the integrand, $\delta X_{ij}(0)$, $i = 2, ... N$, $j = 1, ... 4$ and $\delta X_{ij}(W_i)$, $i = 1,2,3,4$, $j = 1,2, ... 5$. Therefore eliminate these terms from the expression for $\delta \epsilon$, by removing some of the arbitrariness and making them to satisfy the following equations:

$$\dot{\lambda}_{ij} + \sum_{k=1}^{5} \lambda_{ik} \frac{\partial f_{ik}}{\partial X_{ij}} = 0 \quad i = 1,2, ... N$$
$$j = 1,2, ... 5 \quad (4.15)$$

$$\lambda_{ij}(W_i) + \nu_{ij} + \frac{\partial \epsilon}{\partial X_{ij}(W_i)} = 0 \quad i = 1,2, ... N-1$$
$$j = 1,2,3,4 \quad (4.16)$$

$$\lambda_{ij}(0) + \nu_{i-1,j} - \frac{\partial \varepsilon}{\partial X_{ij}(0)} = 0 \quad i = 1,\dots N-1$$

$$j = 1,\dots 4 \quad (4.17)$$

$$\lambda_{i5}(W_i) + \frac{\partial \varepsilon}{\partial W_{i5}(W_i)} = 0 \quad \dots \quad i = 1,2,\dots N-1 \quad (4.18)$$

$$\lambda_{Nj}(W_N) + n_1 \frac{\partial g_1}{\partial X_{Nj}(W_N)} + n_2 \frac{\partial g_2}{\partial X_{Nj}(W_N)}$$

$$+ \frac{\partial \varepsilon}{\partial X_{Nj}(W_N)} = 0 \quad j = 1,2,\dots 5 \quad (4.19)$$

Combining equations (4.16) and (4.17)

$$\lambda_{ij}(W_i) = \lambda_{i+1,j}(0) - \frac{\partial \varepsilon}{\partial X_{i+1,j}(0)} - \frac{\partial \varepsilon}{\partial X_{ij}(W_i)}$$

$$i = 1,2,\dots N-1$$

$$j = 1,2,3,4 \quad (4.20)$$

Equations obtained from (4.15) for the indicated set of i and j are termed as adjoint equations.

Making use of equations (4.8), (4.15) to (4.19), $\delta\varepsilon$ can be written as,

$$\delta\varepsilon = \sum_{l=1}^{N} (\frac{\partial \varepsilon}{\partial W_l} + \sum_{k=1}^{5} \lambda_{lk}(W_l) f_{lk}(W_l)) \delta W_l$$

$$+ \sum_{l=1}^{N} (\frac{\partial \varepsilon}{\partial X_{15}(0)} - \lambda_{15}(0)) \delta X_{15}(0) \quad (4.21)$$

And since δg_1 and δg_2 are assumed to be zero,

$$\sum_{k=1}^{5} \frac{\delta g_1}{\delta X_{Nk}} \delta X_{Nk}(W_N) = 0 \tag{4.22}$$

$$\sum_{k=1}^{5} \frac{\delta g_2}{\delta X_{Nk}} \delta X_{Nk}(W_N) = 0 \tag{4.23}$$

PROCEDURE:

The optimum for the objective function ε can now be approached numerically by using the method of steepest descent. In this method one starts with an arbitrary decision variable vector and approach the optimum by moving in the gradient directions, which are in the direction of minimum. Thus find $\delta \varepsilon$ such that

$$\varepsilon_{new} < \varepsilon_{old}$$

or $$\delta \varepsilon < 0 \tag{4.24}$$

This condition (Equation 4.24) which is also necessary condition for minimum, can be met for (4.21), if

$$\delta W_1 = - w^* \left(\frac{\delta \varepsilon}{\delta W_1} + \sum_{k=1}^{5} \lambda_{1k}(W_1) f_{1k}(W_1) \right) \tag{4.25}$$

$$\delta X_{15}(0) = - w^* \left(\frac{\delta \varepsilon}{\delta X_{15}(0)} - \lambda_{15}(0) \right) \tag{4.26}$$

where w^* is a positive weight function.

Then the potential computational scheme will be as follows:

1. For assumed values of various variables which satisfy the system constraints, calculate coefficients of δW_1 and $\delta X_{15}(0)$ for equation (4.21), by solving equations (4.4) and (4.15) together with conditions (4.8), (4.9), (4.18) to (4.20), (4.22) and (4.23).

2. If constraints are violated, decrease the value of w^* such that $w^* > 0$ and all constraints are satisfied.

3. Now define W_1 and $X_{15}(0)$ such that,

$$W_1|_{new} = W_1|_{old} - w^* \left(\frac{\partial \epsilon}{\partial W_1} + \sum_{k=1}^{5} \lambda_{1k}(W_1) f_{1k}(W_1) \right)$$

$$X_{15}(0)|_{new} = X_{15}(0)|_{old} - w^* \left(\frac{\partial \epsilon}{\partial X_{15}(0)} - \lambda_{15}(0) \right)$$

Repeat steps 1,2 and 3 for new values of W_1 and $X_{15}(0)$ untill no further improvement is possible in ϵ.

It may appear that the coefficients of δW_1 and $\delta X_{15}(0)$ in equations (4.21) can be calculated by integrating the equations (4.4) and (4.15), and making use of equations (4.22) and (4.23) together with initial condition and boundary condition (4.18) through (4.20). But, n_1 and n_2 in equation (4.19) cannot be calculated directly by any of the above equations. As in general cases, one can decide to assume certain values for n_1 and n_2 and check whether relations (4.22) and (4.23)

are satisfied after integrating (4.15) and (4.4). In this case one may have to search over the whole range of n_1 and n_2 to satisfy (4.22) and (4.23), because the system of equations do not give any scheme to improve upon the assumed values. The problem is simplified by using Green's function and Green's identity (15) for both Adjoint equations and variational system equations.

Defining Green's function r_{ijk} for Adjoint equations (4.15) by,

$$\dot{r}_{ijk} = \sum_{l=1}^{5} r_{ijl} \frac{\partial f_{ij}}{\partial X_{il}} \qquad \begin{aligned} &i = 1,2,\ldots N \\ &j \text{ and } k = 1,2,\ldots 5 \end{aligned}$$

(4.27)

with initial conditions

$$r_{ijk}(0) = \delta_{jk}$$

i.e. $\quad r_{ijk}(0) = 1 \quad j = k$

$\qquad\qquad\quad = 0 \quad j \neq k$

The Green's identity for set of equations (4.27) is,

$$\lambda_{ij}(0) = \sum_{k=1}^{5} r_{ijk}(W_i) \lambda_{ik}(W_i) \qquad (4.28)$$

From (4.19) one has,

$$
\begin{bmatrix}
\lambda_{N1}(W_N) \\
\lambda_{N2}(W_N) \\
\vdots \\
\lambda_{N5}(W_N)
\end{bmatrix}
=
\begin{bmatrix}
\dfrac{\partial g_1}{\partial X_{N1}} & \dfrac{\partial g_2}{\partial X_{N1}} & \dfrac{\partial \varepsilon}{\partial X_{N1}} \\
\dfrac{\partial g_1}{\partial X_{N2}} & \cdot & \dfrac{\partial \varepsilon}{\partial X_{N2}} \\
\vdots & \vdots & \vdots \\
\dfrac{\partial g_1}{\partial X_{N5}} & \dfrac{\partial g_2}{\partial X_{N5}} & \dfrac{\partial \varepsilon}{\partial X_{N5}}
\end{bmatrix}
\begin{bmatrix}
-n_1 \\
-n_2 \\
\vdots \\
-1
\end{bmatrix}
\qquad (4.29)
$$

and from (4.28),

$$
\begin{bmatrix}
\lambda_{N1}(0) \\
\lambda_{N2}(0) \\
\vdots \\
\lambda_{N5}(0)
\end{bmatrix}
=
\begin{bmatrix}
\Gamma_{N11} & \Gamma_{N12} & \cdots & \Gamma_{N15} \\
\Gamma_{N21} & & \cdots\cdots & \Gamma_{N25} \\
\vdots & & & \vdots \\
\Gamma_{N51} & & \cdots\cdots & \Gamma_{N55}
\end{bmatrix}
\cdot
\begin{bmatrix}
\lambda_{N1}(W_N) \\
\lambda_{N2}(W_N) \\
\vdots \\
\lambda_{N5}(W_N)
\end{bmatrix}
\qquad (4.30)
$$

Now making use of (4.30) and (4.29), (4.20) gives,

$$
\begin{bmatrix}
\lambda_{N-1,1}(W_{N-1}) \\
\lambda_{N-1,2}(W_{N-1}) \\
\vdots \\
\lambda_{N-1,5}(W_{N-1})
\end{bmatrix}
=
\begin{bmatrix}
\lambda_{N1}(0) \\
\lambda_{N2}(0) \\
\vdots \\
\lambda_{N5}(0)
\end{bmatrix}
-
\begin{bmatrix}
\dfrac{\partial \varepsilon}{\partial X_{N1}}(0) \\
\dfrac{\partial \varepsilon}{\partial X_{N2}}(0) \\
\vdots \\
\dfrac{\partial \varepsilon}{\partial X_{N5}}(0)
\end{bmatrix}
-
\begin{bmatrix}
\dfrac{\partial \varepsilon}{\partial X_{N-1,1}}(W_{N-1}) \\
\dfrac{\partial \varepsilon}{\partial X_{N-1,2}}(W_{N-1}) \\
\vdots \\
\dfrac{\partial \varepsilon}{\partial X_{N-1,5}}(W_{N-1})
\end{bmatrix}
$$

$$
\qquad (4.31)
$$

$$
=
\begin{bmatrix}
A_{11} & A_{12} & A_{13} \\
A_{21} & \cdot & A_{23} \\
\vdots & \vdots & \vdots \\
A_{51} & A_{52} & A_{53}
\end{bmatrix}
\begin{bmatrix}
n_1 \\
n_2 \\
\vdots \\
1
\end{bmatrix}
$$

and it is readily seen that A_{ij} can be expressed in terms of coefficients of, first matrix of right hand side of (4.29), first matrix of right hand side of (4.30) and second and third matrices of right hand side of (4.31).

With the above procedure other values of $\lambda_{ij}(0)$ and $\lambda_{ij}(W_i)$ can be known in terms of n_1 and n_2 and thus coefficients of $\delta X_{15}(0)$ and δW_1 in (4.19) can be known in terms of n_1 and n_2.

Now to calculate values of $\delta X_{Nj}(W_N)$ in terms of n_1 and n_2 which will be used to evaluate n_1 and n_2 from equations (4.22) and (4.23), one writes Green's functions for the Variational System Equation;

$$\mathring{r}_{ijk} = - \sum_{l=1}^{5} r_{ijl} \frac{\partial f_{il}}{\partial X_{ij}} \qquad i = 1,2,\ldots N \qquad '(4.32)$$
$$j \text{ and } k = 1,2,\ldots 5$$

with boundary conditions

$$r_{ijk}(W_i) = 1 \qquad j = k$$
$$= 0 \qquad j \neq k$$

Greens identity for (4.32) is,

$$\delta X_{ij}(W_i) = \sum_{k=1}^{5} r_{ijk}(0)\, \delta X_{ik}(0) \qquad (4.33)$$

And since there is also a δW_1 change in weight of catalyst W_1,

$$
\begin{bmatrix} \delta X_{11}(W_1) \\ \delta X_{12}(W_1) \\ \cdot \\ \cdot \\ \delta X_{14}(W_1) \end{bmatrix}
=
\begin{bmatrix} r_{111} & r_{112} & \cdots & r_{115} \\ r_{121} & \cdot & & \cdot \\ & \cdot & \cdot & \cdot \\ & \cdot & \cdot & \cdot \\ r_{141} & r_{142} & & r_{145} \end{bmatrix}
\begin{bmatrix} \delta X_{11}(0) \\ \delta X_{12}(0) \\ \cdot \\ \cdot \\ \delta X_{15}(0) \end{bmatrix}
+
\begin{bmatrix} f_{11} \cdot \delta W_1 \\ f_{12} \cdot \delta W_1 \\ \cdot \\ ; \\ f_{14} \cdot \delta W_1 \end{bmatrix}
$$

$$
=
\begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ B_{41} & B_{42} & B_{43} \end{bmatrix}
\begin{bmatrix} \eta_1 \\ \eta_2 \\ \\ 1 \end{bmatrix}
$$

Here again coefficients B_{ij} can be easily calculated.

Making use of (4.9) and following the above procedure $\delta X_{Nj}(W_N)$ can be calculated in terms of η_1 and η_2. And now substituting the values of $\delta X_{Nj}(W_N)$ in (4.22) and (4.23), η_1 and η_2 can be calculated.

CHAPTER V

RESULTS AND DISCUSSION

In Table I, the outputs from the model are compared with those from the two industrial plants. The details of each plant e.g., weight of catalyst in each reactor, feed and recycle gas composition, feed rate, recycle ratio, and temperatures and pressure of inlet streams are given in Appendices A and B. Though not all the desired data is available for the industrial reactors, comparison was made with two types of industrial units. One unit has three reactors in series and the other has four reactors in series. The amount of aromatics and paraffins in stream leaving the reactor were predicted with in 7.7 percent and 4.7 percent respectively for the two cases. The temperature of exit streams were also predicted by the model within 1.8 percent. Production rate of hydrogen and hydrocracked products were predicted with in 2.1 percent. The prediction of naphthenes conversion was not satisfactory. A vain attempt was made to increase the accuracy of the results, by changing the rate constants appearing in equations (3.5) through (3.8). However, as the significant characteristics of the reactor systems have been predicted satisfactorily, it can be assumed that the proposed model represents very well the true behaviour of the plants.

TABLE I: SIMULATION RESULT, COMPARISON OF INDUSTRIAL
AND PREDICTED VALUES.

$$I_A \text{ and } I_B = \text{Industrial}$$
$$P = \text{Predicted}$$
$$E = \text{Error } \%$$

Reactor Set-up		Stream leaving reactor	Aromatics lb m/hr	Naphthenes lb m/hr	Paraffins lb m/hr	H$_2$ produced lb m/hr	Hydro-cracked product lb m/hr	Temperature °R
Three in Series	1	I_A						1255.
		P						1288.9
		E						1.3
	2	I_A						1320.
		P						1330.
		E						.8
	3	I_A	170.	8.9	76.5			1400.
		P	157.	2.5	77.4			1374.5
		E	7.7	73.0	1.2			1.8
Four in Series	1	I_B	74.7	80.0	76.0			1271.
		P	73.9	79.31	77.			1281.
		E	1.1	.9	1.3			.8
	2	I_B	109.	39.6	79.2			1318.
		P	108.	38.	82.			1322.
		E	.7	4,0	3.5			.3
	3	I_B	129.4	12.7	75.0			1368.
		P	126.	11.55	78.5			1380.
		E	2.6	10.0	4.7			.9
	4	I_B	140.1	4.9	42.5	252.	122.5	1409.
		P	137.6	5.07	45.6	244.6	119.9	1406.
		E	1.7	21.8	.73	2.1	2.1	.2

The profiles of conversions to aromatics, hydrogen and hydrocracked products and temperature for the plant of Appendix A are shown in Figures 2,3 and 4. It can be seen that in reactor 1 and 2, dehydrogenation of naphthenes to aromatics is dominant (Figures 2 and 3) and since this reaction is endothermic, temperature along the reactor length goes down. It can also be seen from Figure 3 that in reactor -2 more of hydrocracked product is formed than in reactor -1 because of high operating temperature in the reactor-2. Production of aromatics in the reactor -2 is less than in the reactor -1, because dehydrogenation of naphthenes to aromatics is reaching equilibrium, even though the temperature of inlet stream and average operating temperature are higher for reactor -2.

From Figure 4, it can be seen that the conversion of hydrocracked product is dominant and that production of aromatics in very slow in reactor -3. One might expect the temperature to go up and concentration of hydrogen to go down. But the results are contrary. The reaction (2.2), which is endothermic and consumes hydrogen in the forward direction, actually takes place in the backward direction in this reactor. For example extent of reaction (2.2) at the entrance of reactor -3 is .000526 and at the exit it is -.008788.
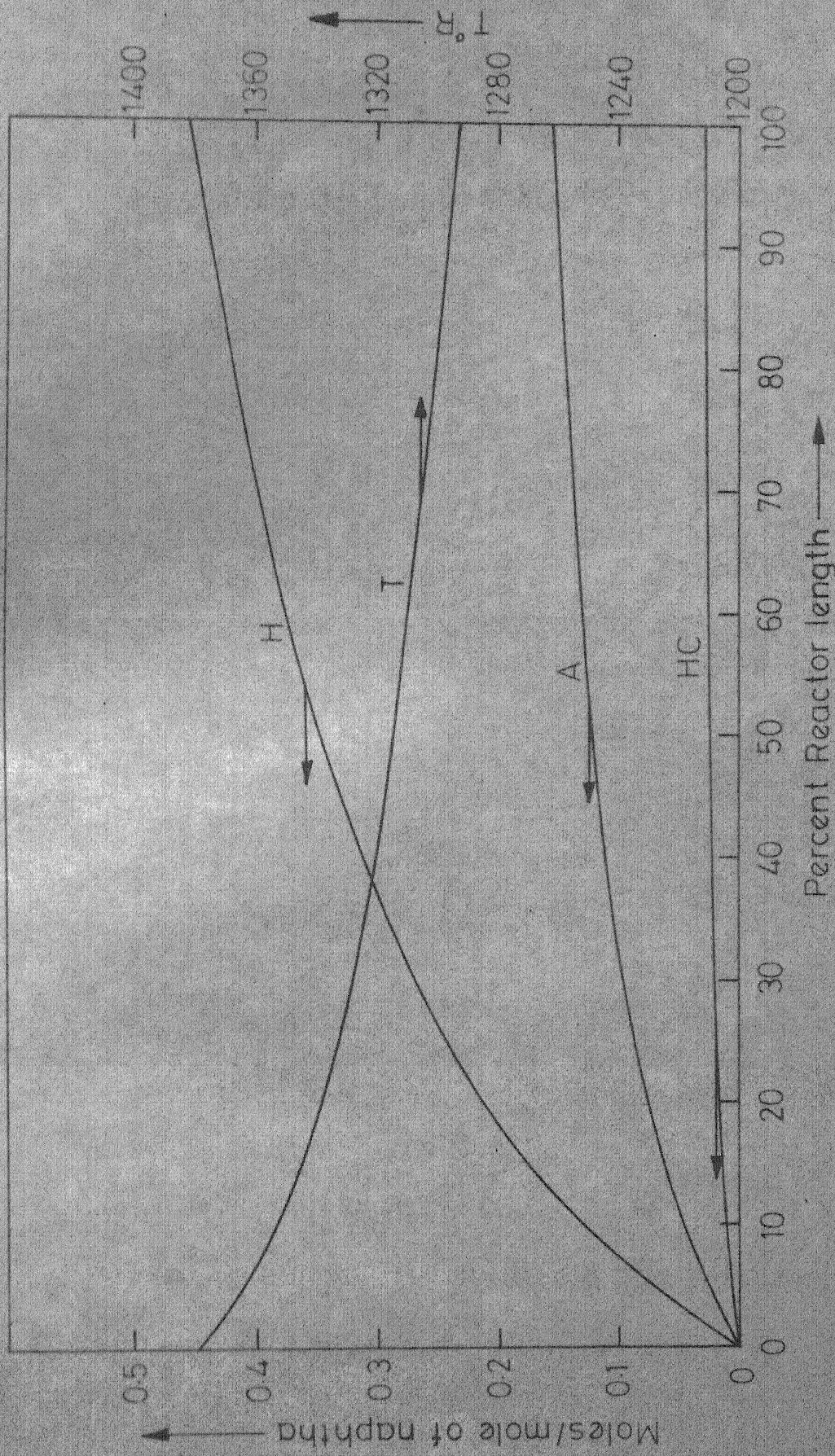
Fig. 2 – Profiles of, aromatics, hydrogen and hydrocracked products produced, and temperature for Reactor 1.
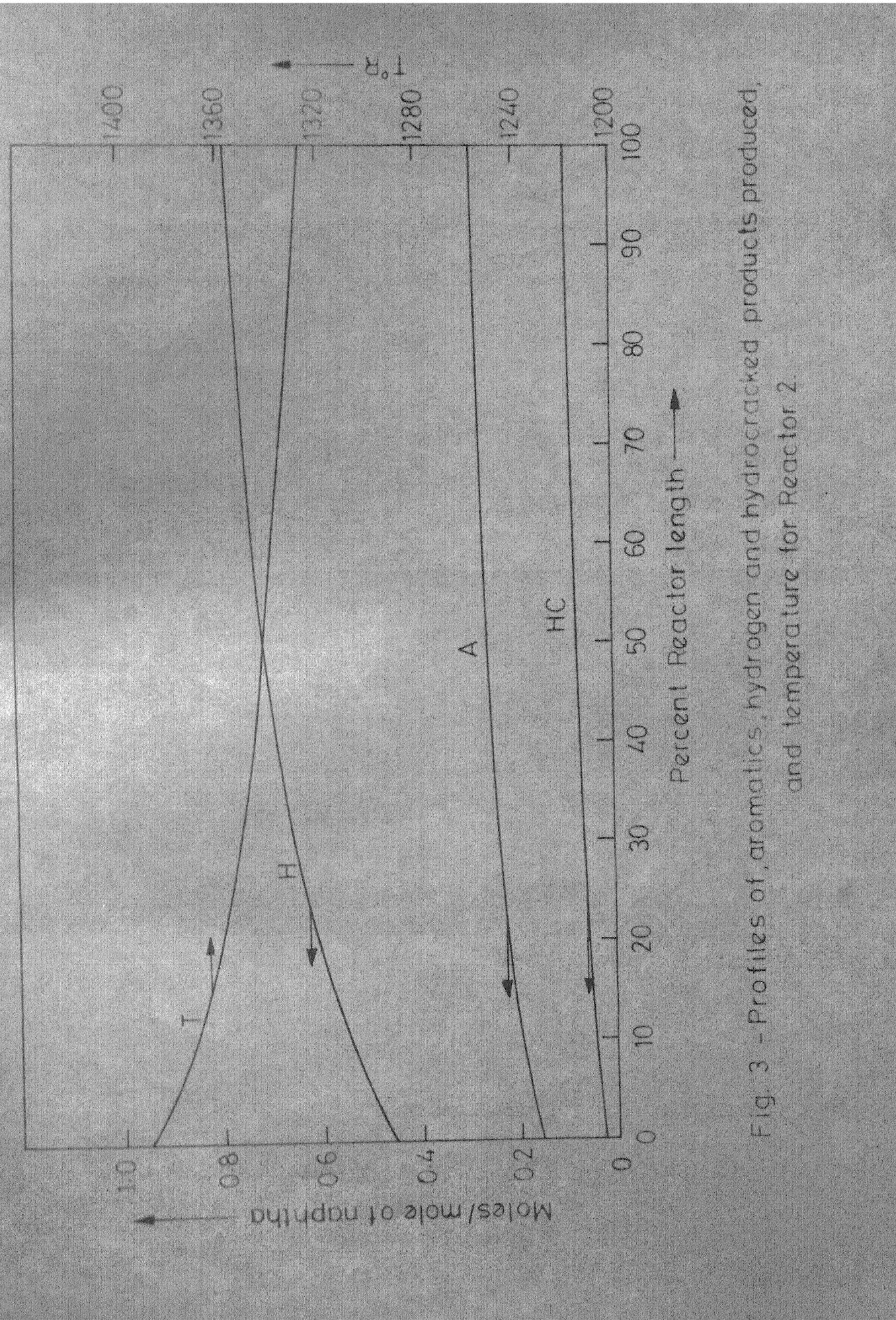
Fig. 3 — Profiles of aromatics, hydrogen and hydrocracked products produced, and temperature for Reactor 2
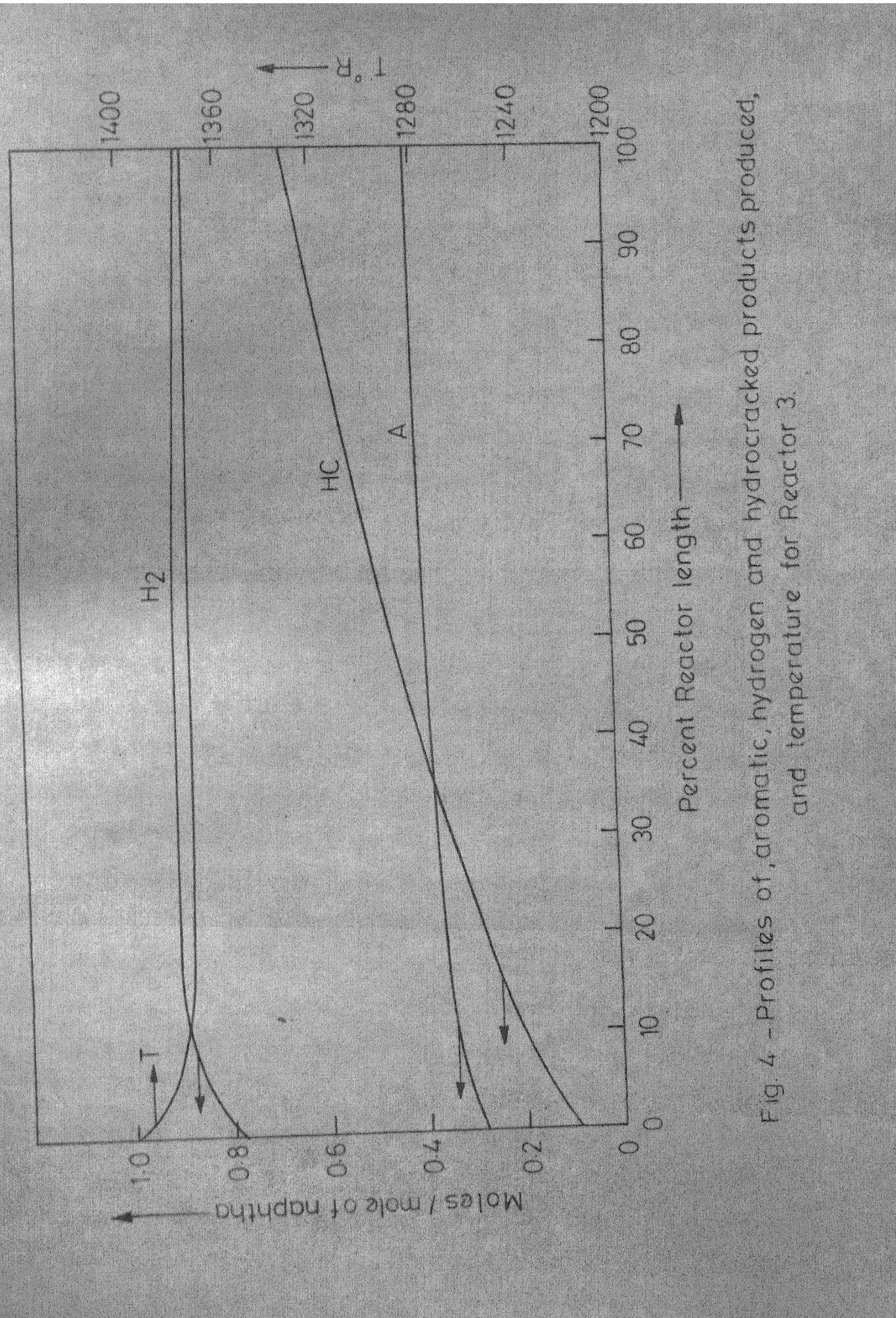
Fig. 4. - Profiles of, aromatic, hydrogen and hydrocracked products produced, and temperature for Reactor 3.

SIMULATION RESULTS:

The simulation model was used to study the effect of recycle ratio, and pressure on the production of aromatics. The results are presented in Figures 5 and 6. The effect of the inlet temperatures of the streams on the production of aromatics, hydrogen and hydrocracked product were also studied. The results are given in Table II and Figures 7, 8 and 9. Additional plant data is taken from Appendix A.

(i) Effect of Recycle Ratio:

It can be seen from Figure 5 that as the recycle ratio rises, from 3 to 8, the production of aromatics also rises from .3336 to .4018 mole of aromatics per mole of naphtha, and as it increases from 8 to 10 the production of aromatics remains almost steady. Since reaction (2.1) produces hydrogen in the forward direction, one can expect that the aromatic production rate will go down with the rise in recycle ratio, as the increase in its value increases the partial pressure of hydrogen. But the results are contrary. As the hydrogen partial pressure in the reaction mixture rises because of rise in the recycle ratio, the exothermic reaction (2.2) becomes fast. The temperature rise because of more heat produced in reaction (2.2) is sufficient enough to off set the decrease in the reaction rate of reaction (2.1). It can be further noted from Figure 5 that as recycle ratio rises,
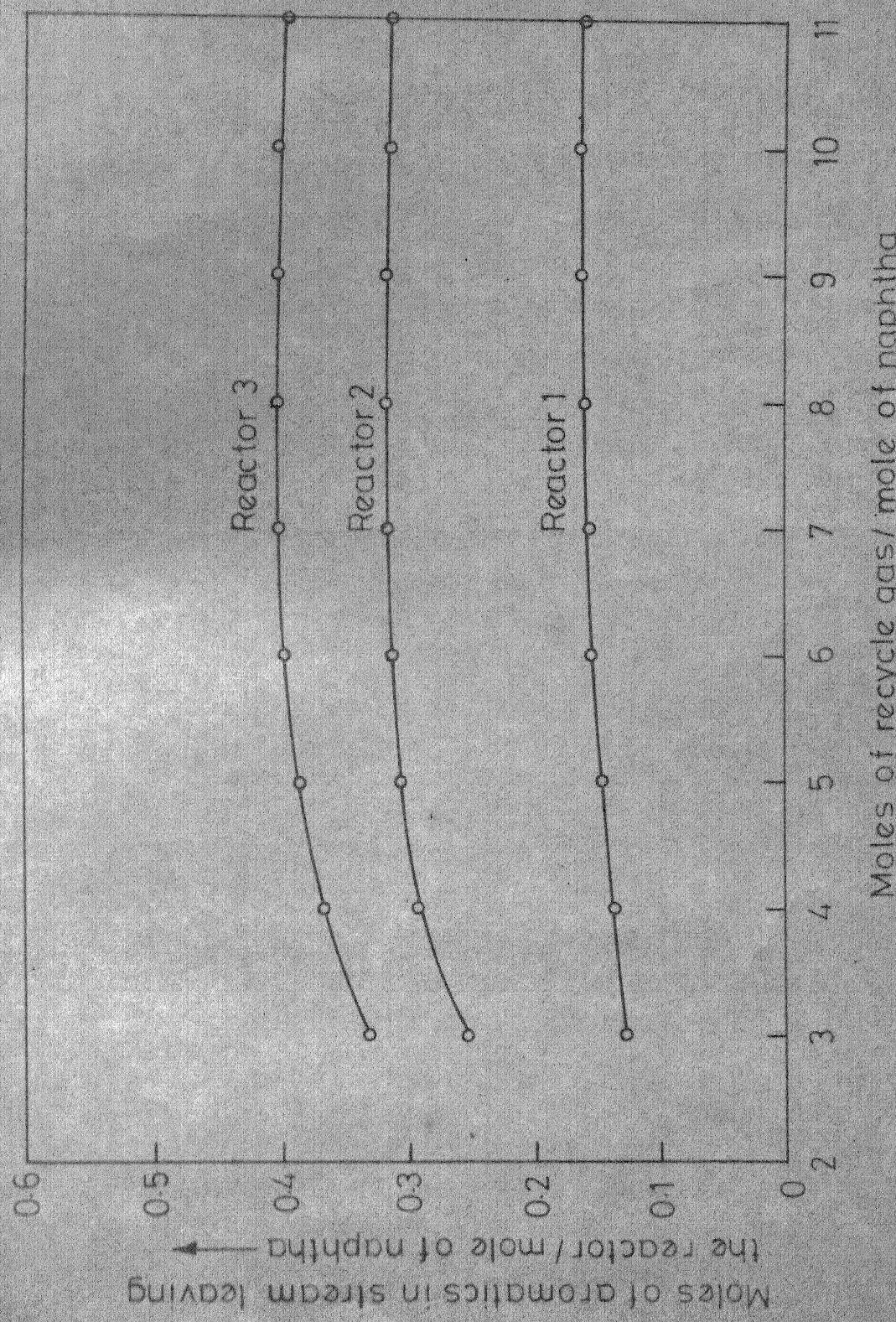
Fig 5 – Effect of recycle ratio on yield of aromatics.
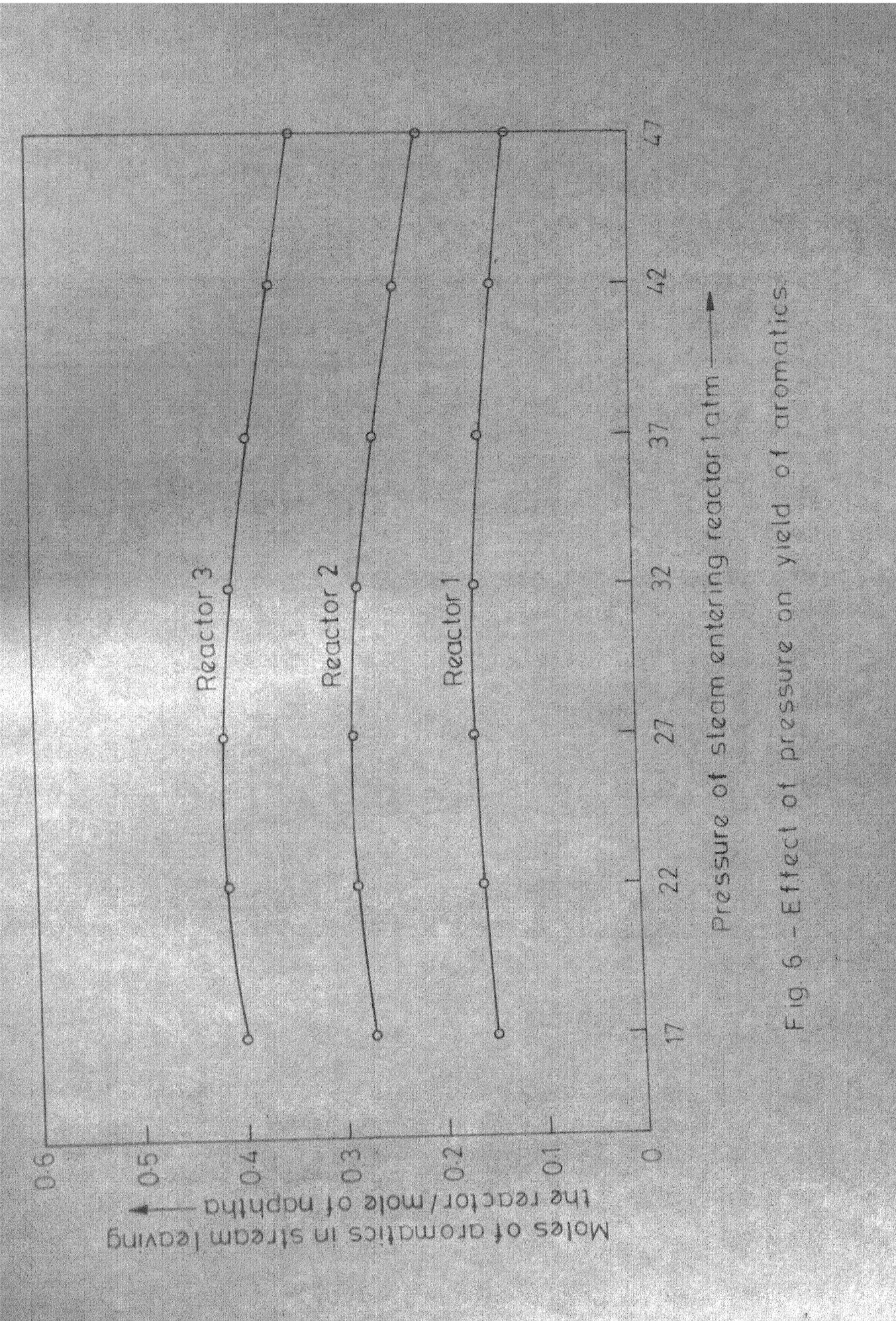
Fig. 6.– Effect of pressure on yield of aromatics

TABLE II: EFFECT OF TEMPERATURE ON CONVERSION OF
AROMATICS, HYDROGEN AND HYDROCRACKED
PRODUCTS.

T_1	Conver- sion in Reactor 1	T_2	Conver- sion in Reactor 2	Conversion in Reactor 3 for					
				$T_3=$ 1285.	$T_3=$ 1320.	$T_3=$ 1355.	$T_3=$ 1390.	$T_3=$ 1425.	$T_3=$ 1460.
1285.	.0559 .1644 .0032	1285.	.1093 .3209 .0072	.1978 .5764 .0192	.2381 .6882 .0315	.2759 .7846 .0561	.3093 .8516 .1087	.3384 .8660 .2366	.3834 .8014 .6074
		1320.	.1437 .4191 .0129	.2201 .6372 .0268	.2585 .7423 .0413	.2937 .8282 .0718	.3243 .8791 .1406	.3553 .8762 .3169	.4123 .8167 .7647
		1355.	.1824 .5251 .0248	.2437 .6868 .0414	.2795 .7921 .0599	.3113 .8630 .1009	.3399 .8938 .2005	.3785 .8772 .4575	.4461 .8309 .9539
		1390.	.2228 .6280 .0484	.2663 .7442 .0691	.2986 .8259 .0942	.3270 .8775 .1549	.3575 .8884 .3107	.4101 .8689 .6682	.4748 .8382 1.1223
		1425.	.2626 .7135 .0948	.2857 .7660 .1216	.3141 .8305 .1585	.3409 .8615 .2541	.3801 .8604 .4839	.4438 .8494 .9107	.4888 .8280 1.2247
		1460.	.2991 .7597 .1907	.3014 .7462 .2250	.3264 .7931 .2786	.3555 .8090 .4220	.4052 .8077 .7342	.4654 .8072 1.1121	.4867 .7883 1.2731
1320.	.0910 .2649 .0079	1285.	.1375 .4009 .0120	.2160 .6257 .0255	.2548 .7321 .0396	.2904 .8199 .0689	.3215 .8738 .1344	.3520 .8736 .3010	.4069 .8126 .7370
		1320.	.1701 .4936 .0181	.2364 .6807 .0337	.2731 .7795 .0508	.3060 .8556 .8780	.3351 .8930 .1756	.3705 .8799 .4038	.4357 .8287 .8925
		1355.	.2069 .5935 .0310	.2580 .7335 .0499	.2918 .8214 .0719	.3216 .8815 .1230	.3506 .9002 .2518	.3911 .8804 .5684	.4653 .8435 1.0546
		1390.	.2451 .6888 .0572	.2783 .7729 .0809	.3086 .8463 .1114	.3359 .8874 .1877	.3702 .8909 .3843	.4298 .8747 .7832	.4865 .8474 1.1762
		1425.	.2822 .7639 .1103	.2958 .7860 .1406	.3226 .8427 .1848	.3502 .8662 .3016	.3948 .8637 .5802	.4593 .8577 .9946	.4936 .8379 1.2386
		1460.	.3161 .7955 .2234	.3113 .7596 .2601	.3356 .8017 .3198	.3560 .8149 .4782	.4179 .8153 .8018	.4738 .8173 1.1487	.4890 .7988 1.2709

T_1	Conversion in Reactor 1	T_2	Conversion in Reactor 2	Conversion in Reactor 3 for					
				$T_3=$ 1285.	$T_3=$ 1320.	$T_3=$ 1355.	$T_3=$ 1390.	$T_3=$ 1425.	$T_3=$ 1460.
		1285.	.1692	.2355	.2721	.3050	.3340	.3695	.4348
			.4873	.6743	.7729	.8487	.8858	.8724	.8214
			.0217	.0374	.0544	.0916	.1798	.4091	.8983
		1320.	.1994	.2535	.2878	.3182	.3469	.3911	.4598
			.5724	.7216	.8117	.8748	.8968	.8774	.8479
			.0284	.0466	.0675	.1155	.2354	.5356	1.0290
1355.	.1310 .3763 .0175	1355.	.2334	.2723	.3038	.3317	.3637	.4198	.4818
			.6638	.7656	.8438	.8908	.8981	.8798	.8519
			.0429	.0649	.0925	.1597	.3333	.7124	1.1440
		1390.	.2686	.2900	.3183	.3454	.3857	.4503	.4943
			.7485	.7953	.8588	.8888	.8874	.8772	.8561
			.0732	.1008	.1391	.2386	.4865	.9077	1.2143
		1425.	.3024	.3058	.3313	.3606	.4105	.4726	.4961
			.8096	.7991	.8477	.8648	.8632	.8621	.8430
			.1369	.1713	.2246	.3666	.6779	1.0706	1.2461
		1460.	.3343	.3231	.3468	.3779	.4298	.4802	.4907
			.8238	.7686	.8072	.8189	.8212	.8246	.8068
			.2782	.3162	.3796	.5461	.8670	1.1766	1.2685
		1285.	.2022	.2541	.2880	.3178	.3467	.3927	.4611
			.5700	.7126	.8006	.8610	.8800	.8600	.8228
			.0405	.0592	.0810	.1316	.2591	.5734	1.0607
		1320.	.2291	.2691	.3007	.3286	.3604	.4159	.4785
			.6455	.7507	.8295	.8772	.8851	.8664	.8380
			.0479	.0697	.0968	.1627	.3300	.7087	1.1454
1390.	.1738 .4883 .0361	1355.	.2596	.2849	.3137	.3408	.3792	.4429	.4914
			.7253	.7843	.8509	.8842	.8838	.8715	.8496
			.0647	.0911	.1269	.2189	.4512	.8704	1.2068
		1390.	.2909	.3000	.3263	.3547	.4023	.4669	.4968
			.7960	.8035	.8566	.8770	.8746	.8709	.8515
			.1015	.1340	.1826	.3118	.6103	1.0214	1.2372
		1425.	.3210	.3152	.3397	.3709	.4242	.4809	.4961
			.8394	.7996	.8414	.8544	.8550	.8574	.8387
			.1826	.2208	.2827	.4467	.7787	1.1299	1.2521
		1460.	.3534	.3379	.3608	.3908	.4396	.4839	.4913
			.8377	.7703	.8075	.8192	.8228	.8265	.8096
			.3685	.4051	.4667	.6271	.9265	1.1968	1.2677

T_1	Conversion in Reactor 1	T_2	Conversion in Reactor 2	Conversion in Reactor 3 for					
				$T_3=$ 1285.	$T_3=$ 1320.	$T_3=$ 1355.	$T_3=$ 1390.	$T_3=$ 1425.	$T_3=$ 1460.
			.2344	.2701	.3006	.3278	.3612	.4198	.4779
		1285.	.6380	.7296	.8041	.8464	.8505	.8335	.8079
			.0763	.0993	.1288	.2021	.3916	.7848	1.1883
			.2572	.2817	.3102	.3371	.3760	.4400	.4868
		1320.	.7006	.7572	.8225	.8543	.8533	.8417	.8201
			.0847	.1113	.1478	.2419	.4793	.8900	1.2247
			.2829	.2942	.3206	.3488	.3954	.4605	.4925
	.2170	1355.	.7653	.7797	.8340	.8553	.8527	.8481	.8287
1425.	.5890		.1049	.1367	.1837	.3087	.6014	1.0171	1.2459
	.0717		.3095	.3072	.3321	.3629	.4160	.4758	.4942
		1390.	.8180	.7894	.8332	.8471	.8467	.8481	.8292
			.1520	.1894	.2492	.4082	.7404	1.1127	1.2554
			.3370	.3243	.3481	.3799	.4320	.4831	.4930
		1425.	.8424	.7821	.8197	.8309	.8337	.8376	.8198
			.2618	.3012	.3672	.5400	.8674	1.1746	1.2625
			.3751	.3571	.3728	.4056	.4479	.4850	.4902
		1460.	.8335	.7611	.7988	.8117	.8157	.8186	.8032
			.5096	.5413	.5945	.7328	.9898	1.2161	1.2711
			.2640	.2819	.3089	.3358	.3181	.4423	.4799
		1285.	.6748	.7108	.7695	.7947	.7921	.7844	.7643
			.1464	.1749	.2160	.3244	.5887	1.0037	1.2686
			.2814	.2901	.3158	.3441	.3919	.4554	.4833
		1320.	.7214	.7278	.7790	.7978	.7953	.7923	.7731
			.1559	.1883	.2375	.3689	.6698	1.0733	1.2759
			.3013	.2996	.3242	.3548	.4077	.4672	.4854
	.2584	1355.	.7669	.7402	.7835	.7969	.7964	.7979	.7792
1460.	.6611		.1810	.2179	.2774	.4361	.7673	1.1379	1.2791
	.1415		.3229	.3121	.3359	.3682	.4225	.4750	.4860
		1390.	.7990	.7438	.7813	.7921	.7944	.7984	.7803
			.2440	.2839	.3510	.5272	.8639	1.1854	1.2809
			.3510	.3348	.3574	.3873	.4359	.4791	.4859
		1425.	.8092	.7397	.7760	.7873	.7911	.7951	.7786
			.3959	.4323	.4943	.6554	.9527	1.2157	1.2825
			.3991	.3791	.3992	.4214	.4544	.4825	.4856
		1460.	.8061	.7315	.7704	.7849	.7891	.7905	.7770
			.7039	.7283	.7690	.8746	1.0723	1.2443	1.2837

How to read the table:

Upper, middle and lower numerical values of the three figures appearing together in the columns of 'conversion in reactor' stand for aromatics, hydrogen and hydrocracked product, produced per mole of naphtha respectively. For example, aromatics, hydrogen and hydrocracked product produced per mole of naphtha in the stream leaving, reactor one for $T_1 = 1285$ are .0559, .1644 and .0032, reactor two for $T_1 = 1285$, $T_2 = 1320$ are .1437, .4191 and .0129, and reactor three for $T_1 = 1285$, $T_2 = 1320$ and $T_3 = 1355$ are .2937, .8282 and .0718.
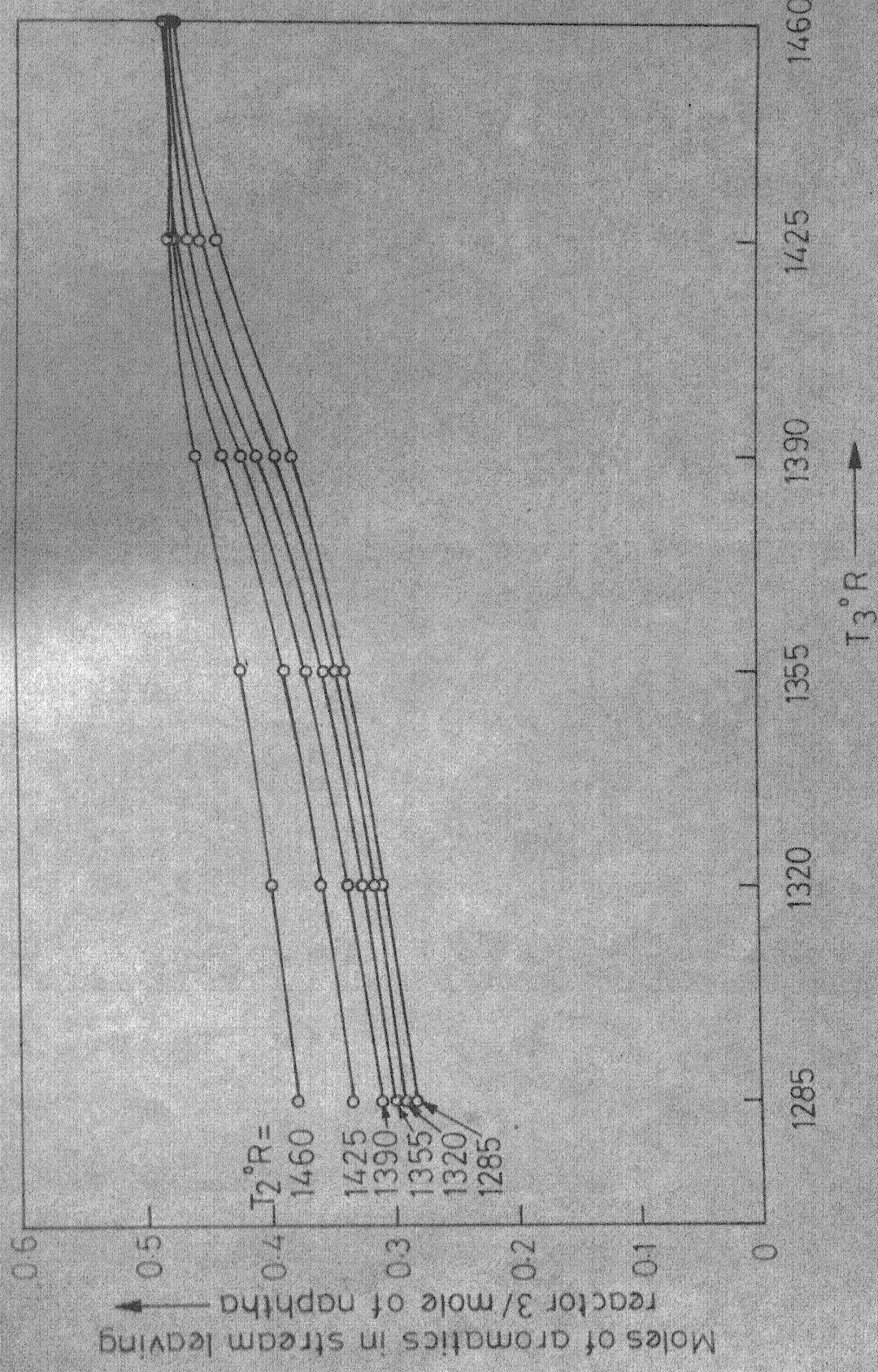
Fig. 7 – Effect of temperature on conversion of aromatics for $T_1 = 1460°R$.

$T_3°R$

Moles of aromatics in stream leaving reactor 3/mole of naphtha

$T_2°R =$
1460
1425
1390
1355
1320
1285
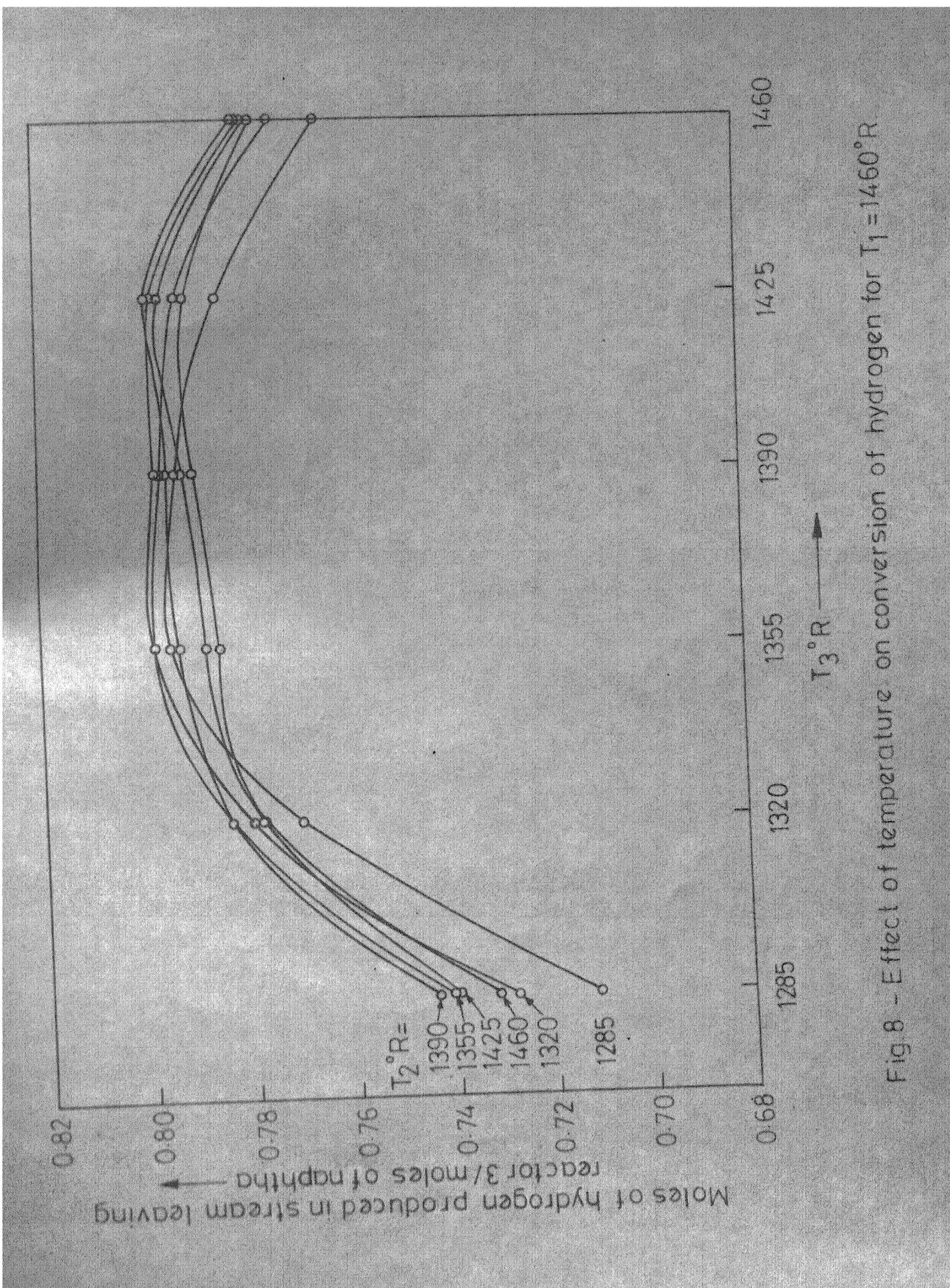
Fig. 8 – Effect of temperature on conversion of hydrogen for $T_1 = 1460°R$.
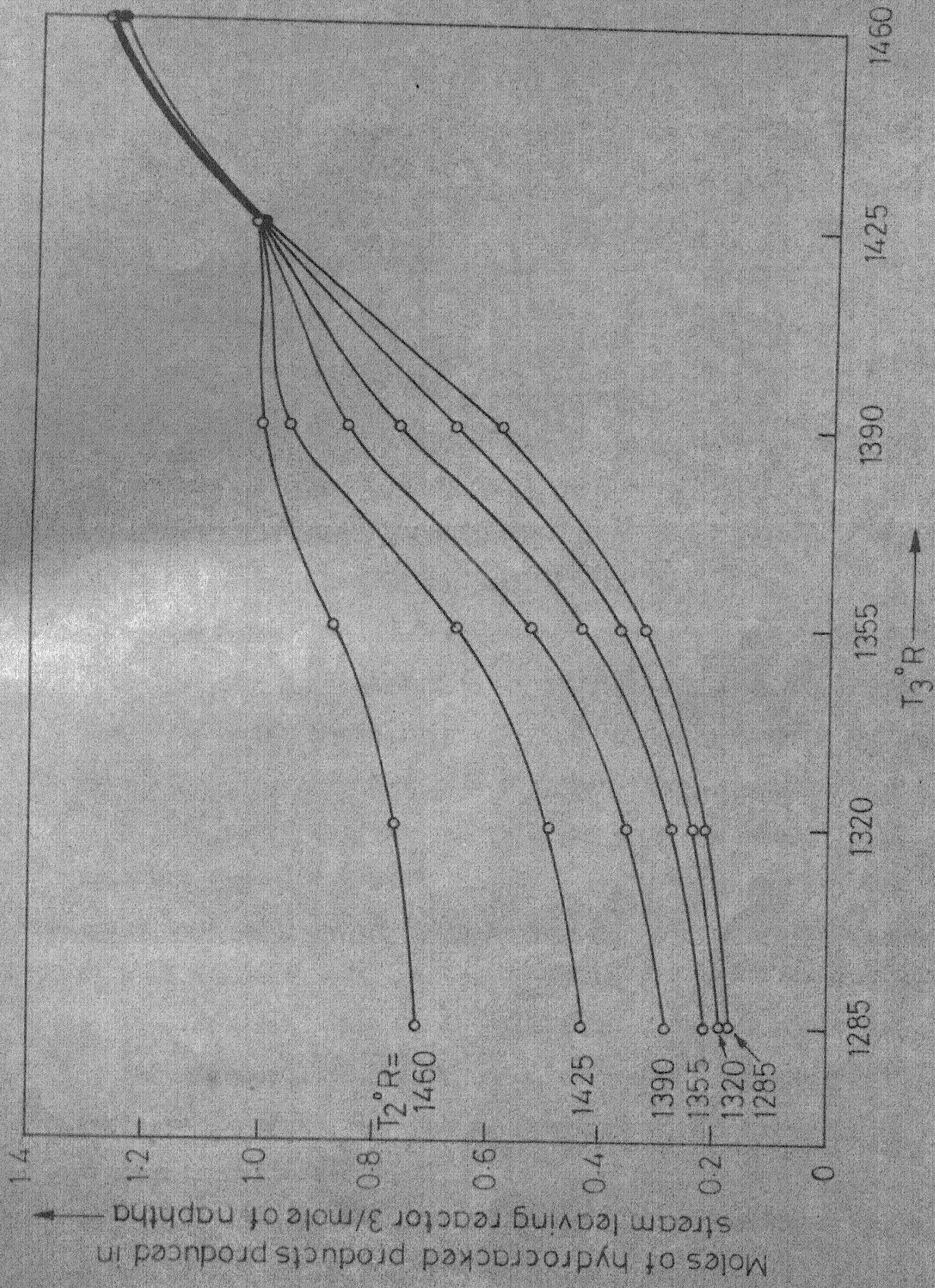
Fig. 9 – Effect of temperature on conversion of hydrocracked products for

the increase in aromatics production rate decreases. At
higher recycle ratio, the effect of extra heat produced
because of reaction (2.2) becoming fast to make the reaction
(2.1) fast, decreases.

(ii) Effect of Pressure:

It can be seen from Figure 6 that as pressure of inlet
stream rises from 17 to 27 atmospheres, the production of
aromatics rises from .3985 to .4131 and then decreases from
.4131 to .3431 moles of aromatics/mole of naphtha as pres-
sure rises from 27 to 47 atmospheres. From the Le Chatellier's,
principle one will expect the production of aromatics to go
down with an increase in pressure, because both in naphthenes
dehydrogenation to aromatics and paraffin dehydrogenation
to naphthenes a rise in number of moles is resulted. As the
pressure rises exothermic reaction (2.2) becomes fast and
leads to a rise in the temperature of reaction mixture, and
at high temperatures, the reaction (2.1) which is endother-
mic becomes fast enough to off set the decrease in the rate
of dehydrogenation of naphthenes to aromatics because of
increase in pressure. But as pressure rises, the rise in
temperature because of (2.2) becoming fast is not sufficient
enough to off-set the effect of the rise in pressure and as
a result the production of aromatics goes down.

(iii) Effect of Temperature:

The effect of temperature on production of aromatics, hydrogen and hydrocracked product is given in Table II and figures 7, 8 and 9. Figures 7, 8 and 9 represent a typical set of curves for one inlet set of temperature for reactor-1. It can be seen from Table II that the amount of aromatics and hydrogen in the stream leaving reactor-1 is approximately a linear function of temperature. The amount of aromatics produced in reactor-2 is also approximately a linear function of T_2 for every value of T_1. The amount of aromatics in the stream leaving the reactor-3 rises with rise in temperature of inlet stream to any reactor except for $T_1 > 1390$, $T_2 > 1355$ and $1425^{\circ}R$.

For the above excepted value a rise in inlet temperatures of all reactors, produces only marginal decrease in production of aromatics.

For $T_1 = 1425$ and $T_2 \geq 1390$, and $T_1 = 1460$ and $T_2 \geq 1355$ amount of aromatics is less in the stream leaving reactor-3 than the stream leaving reactor-2 for $T_3 = 1285$. At the above values of T_1 and T_2, conversion of naphthenes to aromatics is very fast in reactor one and two. The concentration of naphthenes in reaction mixture of reactor-3 for $T_3 = 1285$ is low enough to reverse the direction of reaction (2.1) as this reaction is endothermic. Since reaction (2.2) is exothermic, at low temperature hydrogenation of naphthenes to paraffins is favoured and as a result the concentration of naphthenes is lowered.

It is seen from Fig. 7 that amount of aromatics
produced at T_1 = 1460 and T_3 = 1460 is approximately inde-
pendent of T_2.

As hydrogen takes part in all the reactions, its
production does not follow any pattern (See Figure 8).

The production of hydrocracked products rises with
the rise in temperature of the inlet streams and it is seen
from Figure 9 that it's amount is approximately independent
of T_2 for T_1 = 1460 and T_3 between 1425 and 1460.

OPTIMIZATION:

The procedure outlined in Chapter IV to minimize an
objective function, ϵ, with constraints on temperature and
concentrations of the stream leaving the last reactor of
the series was used to minimize the total weight of catalyst
and operating cost for three, four and five reactors in
series. The respective objective function for total weight
of catalyst and operating cost, and the constraints are given
in Appendix D. The results obtained by computer programme
(see Appendix E) developed in the present study, are given
in Table III and IV (For additional data, please see
Appendix A).

When minimizing the total weight of catalyst and the
operating cost for five reactors in series catalyst weight
for one of these reactors come out to be zero. Though the

TABLE III: RESULTS FOR MINIMIZATION OF WEIGHT
OF CATALYST

SS =   Starting solution

FS =   Final solution

			Reactor					Total wt. of catalyst lb.
			1	2	3	4	5	
Three Reactors	SS	W_i	1500.0	1940.0	13900.0			17340.0
		T_i	1378.8	1389.6	1398.6			
	FS	W_i	327.9	658.7	12437.1			13423.7
		T_i	1402.3	1380.6	1439.5			
Four Reactors	SS	W_i	1500.0	1940.0	6900.0	6900.0		17340.0
		T_i	1378.8	1389.6	1398.6	1375.0		
	FS	W_i	1215.9	1283.4	831.4	1387.0		4717.7
		T_i	1402.9	1433.1	1460.0	1408.7		
Five Reactors	SS	W_i	1500.0	1940.0	4633.3	4633.3	4633.3	17340.0
		T_i	1378.8	1389.6	1398.6	1375.0	1374.0	
	FS	W_i	0.0	472.8	3241.7	3242.7	3263.8	10221.0
		T_i	1366.0	1366.0	1391.5	1438.9	1372.6	

TABLE IV: RESULTS FOR MINIMIZATION OF OPERATING COST

SS = Starting solution
FS = Final solution

			Reactor					Operating cost in lakhs of Rs. per year
			1	2	3	4	5	
Three Reactor	SS	W_i	1500.0	1940.0	13900.0			32.36
		T_i	1378.8	1389.6	1398.6			
	FS	W_i	1159.7	1459.8	12858.2			29.44
		T_i	1367.7	1391.7	1410.3			
Four Reactor	SS	W_i	1500.0	1940.0	6900.0	6900.0		32.22
		T_i	1378.8	1389.6	1398.6	1375.0		
	FS	W_i	1967.8	2036.2	1445.3	2336.6		17.75
		T_i	1355.2	1373.0	1406.7	1429.3		
Five Reactor	SS	W_i	1500.0	1940.0	4633.3	4633.3	4633.3	32.39
		T_i	1378.8	1389.6	1398.6	1375.0	1374.0	
	FS	W_i	2298.7	2462.3	2302.1	0.0	1480.4	19.03
		T_i	1357.0	1375.0	1409.9	1360.6	1436.7	

three starting solutions which were tried led to one of W_i going to zero, there can be an initial solution which can avoid such a situation.

Since the iterations were stopped when one of the W_i values went to zero, the final solutions given in Tables III and IV for the five reactors in series do not represent the real optimum. When these values were used as a starting solution for the four reactors in series, approximately the same results were obtained as given in Tables III and IV for four reactor cases.

From the results obtained it is concluded that one should use four reactors in series. But the result can be different if one maximizes for venture profit. In operating cost the number of inter heaters, which depend on the number of reactors being used is not considered but will figure in venture profit.

During computation, it was found necessary to reduce the scale of temperature and naphtha feed rate by factors of 10-40 and 50-100 respectively. It was also found necessary to reduce the scale of optimization function by a factor of 100 when minimizing the operating cost. These scaling were made necessary for, in the development of algorithm, second and higher order terms have been assumed to be negligible as compared to the first order terms. In order to reduce the total

number of iterations., it was found useful to use a lower factor for temperature and a higher for naphtha feed rate initially and then keep changing these factors after some iterations.

The values of constraints g_1 and g_2 were .046 and .5731 respectively at the starting of the iterations for optimization in all the cases considered for the optimization study. These equality constraints were allowed only a change of $\pm$ .0005 and $\pm$ .005 respectively from the starting value. If the change in the values of g_1 and g_2 was more than the above given value, $w*$, the multiplication factor to determine the magnitude of changes in decision variables, which had an initial value 4, was reduced to half each time till the constraints met the prescribed limits.

The iterations were stopped when changes in objective functions for the weight of catalyst and the operating cost were less than 1.0 and 50.0 respectively. For both the objective functions, the time taken on IBM 7044 to reach the final solution from the starting solution were approximately 20, 35 and 15 minutes respectively.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

The mathematical model developed for the catalytic-reforming process predicted very well the temperature and concentration of various components in the exit stream of the reactors, for two different industrial units.

Simulated results show that as recycle ratio rises, the production of aromatics also increases. Maximum production of aromatics occur at a pressure of 27 atmospheres. The rise in temperature of inlet stream increases the production of aromatics and hydrocracked products. From the simulated results, it is recommended that for the plant of Appendix A, the temperatures of inlet streams should be changed to $T_1 = 1390$, $T_2 = 1390$ and $T_3 = 1460$ from the existing values, to increase the production rate of aromatics to 135.2 moles/hr from its present value of 112.2. The increase in temperature will lead to more load on inter heaters. So one has to make an economic evaluation of the process before taking the final decision.

If one wishes to use the minimum weight of catalyst, or to have the minimum operating cost to produce aromatics at a rate, being produced in plant of Appendix A from naphtha (its composition and feed rate are given in Appendix A), one should use four reactors in series.

In the existing plant (Appendix A) one can use less weight of catalyst or operate at lower operating cost for the same aromatic production rate and the same quality of reformate. The weight of catalyst can be reduced by 19.8 per cent (See Table III) and operating cost by 9.05 per cent by changing, the catalyst distribution in the reactors and temperature of inlet streams to the reactors.

RECOMMENDATIONS FOR FURTHER STUDIES:

1.   In the present study, inter heaters have not been included in the simulation. A mathematical model representing the behaviour of inter heaters can be combined with the present simulation model.

2.   Mathematical model representing the flash unit can also be incorporated with the present simulation model.

3.   Recycle ratio and operating pressure can also be used as variables in the optimization function.

4.   For design optimization of Platformer unit, a venture profit concept can be used as an objective function.

BIBLIOGRAPHY

1. Haensel, V., Oil and Gas J., March 30, 1950.

2. Kenneth, A. Kobe, and John, J. Mckentta Jr.,
    Advances in Petroleum Chemistry and Refining,
    Vol. 1, Chapter 8, Interscience Publisher (1958).

3. Smith, R.B., Chemical Engg. Progress, 55, (6)
    p. 74, (1959).

4. Katrush, V.I., Faktorova, R.V., Andrienko,I.E.,
    and Pravenku, A.Ya., Khim Tekhnol Topl. Masel
    16 (4), p. 32 (1971).

5. Hamingsen, J., and Nielson, B., British Chemical
    Engg. 15 (11) p.1433 (1970).

6. Vermorner, M., Faatz, G., and Gelbin, D., Chemical
    Technology (Berlin) 14, p.328 (1962).

7. Nelson, W.N., Petroleum Refinery Engg., McGraw-Hill
    (1958).

8. Kramer, H., and Westerterp, K.R., Elements of
    Chemical Reactor design, p. 225, Academic Press,
    INC (1963).

9. Foust,A.S., Wenzel, L.A., Clump, C.W., Maus, L.,
    and Andersen, L.B., Principles of Unit Operations,
    John Wiley and Sons (1960).

10. Denn, M.M., and Aris, R., I and E C Fundamentals,
    4 (3) p. 213 (1965).

11. Denn, M.M., and Aris, R., I and E C Fundamentals,
    4 (2) p. 248 (1965).

12. Denn, M.M., and Aris, R., AIChE J., 11, p.367 (1965).

13. Douglas, J.M., and Denn, M.M., Industrial Engg.
    Chemistry, 57 (11) p. 18 (1965).

14. Katz, S., I and E C Fundamentals, 1 (3) p. 226 (1962).

15. Denn, M.M., Optimization by Variational Method,
    McGraw-Hill (1969).

APPENDIX A

PLANT DATA FOR THREE REACTORS SET-UP

Feed = 272.2 moles/hr.

Recycle ratio = 7.95

Reactor	Weight of catalyst lb	Temp. of inlet stream °R	Pressure of inlet stream atm.
1	1500	1378.8	22.0
2	1940	1389.6	20.5
3	13900	1398.6	18.6

Naphtha Feed Composition:

C_7-Paraffins	2.2	% by wt.
C_7-Naphthenes	2.9	"
C_7-Aromatics	2.0	"
C_8-Paraffins	29.0	"
C_8-Naphthenes	29.3	"
C_8-Aromatics	12.6	"
C_9-Paraffins	18.4	"
C_9-Naphthenes	3.6	"

Recycle Gas Composition:

Hydrogen	86.0	Mole %
Methane	6.0	"
Ethane	2.8	"
Propane	2.1	"
Butane	1.0	"
Pentane	0.5	"
C_6-Paraffins	0.6	"
C_6-C_8 Hydrocarbons	1.0	"

APPENDIX B

PLANT DATA FOR FOUR REACTORS SET-UP

Feed = 232.8 moles/hr

Recycle ratio = 6.9

Reactor	Weight of catalyst lb	Temperature of inlet stream $^{\circ}R$	Pressure of inlet stream atm.
1	1180	1403	39.9
2	1180	1403	39.5
3	3230	1403	39.1
4	4150	1403	38.1

Naphtha feed composition:

C_6-Paraffins	0.3	% by wt.
C_6-Naphthenes	0.7	"
C_6-Aromatics	0.1	"
C_7-Paraffins	5.9	"
C_7-Naphthenes	9.3	"
C_7-Aromatics	3.7	"
C_8-Paraffins	23.9	"
C_8-Naphthenes	26.1	"
C_8-Aromatics	11.5	"
C_9-Paraffins	15.0	"
C_9-Naphthenes	1.9	"
C_9-Aromatics	1.6	"

Recycle Gas Composition:

Hydrogen	86.4	Mole %
Methane	5.1	"
Ethane	3.6	"
Propane	2.1	"
Butane	1.406	"
Pentane	0.666	"
Hexane and higher	0.698	"

APPENDIX C

HEAT CAPACITIES

Let it be assumed that $SP1_i + SP2_i.T$, $SN1_i + SN2_i.T$, $SA1_i + SA2_i.T$, $SH1 + SH2.T$ are specific heats and; XP_i, XN_i, XA_i, XHI are mole fractions of, paraffins, naphthenes, aromatics and hydrogen in the feed to first reactor where 'i' is number of carbon atoms. And since C_{10} and higher compounds are negligible, the specific heat for various classes of compounds in the feed to first reactor e.g., C_6 and higher paraffins, naphthenes, aromatics and C_5 and lower paraffins, hydrogen and hydrocarbons produced from hydrocracking, can be written as:

$$C_{pP} = \frac{\sum_{i=6}^{9} SP1_i.XP_i}{\sum_{j=6}^{9} XP_i} + \frac{\sum_{i=6}^{9} SP2_i.XP_i}{\sum_{i=6}^{9} XP_i} .T$$

$$C_{pN} = \frac{\sum_{i=6}^{9} SN1_i.XN_i}{\sum_{i=6}^{9} XN_i} + \frac{\sum_{i=6}^{9} SN2_i.XN_i}{\sum_{i=6}^{9} XN_i} . T$$

$$C_{pA} = \frac{\sum_{i=6}^{9} SA1_i.XA_i}{\sum_{i=6}^{9} XA_i} + \frac{\sum_{i=6}^{9} SA2_i.XA_i}{\sum_{i=6}^{9} XA_i} . T$$

$$C_{pHCI} = \frac{\sum\limits_{i=1}^{5} SP1_i \cdot XP_i}{\sum\limits_{i=1}^{5} XP_i} + \frac{\sum\limits_{i=1}^{5} SP2_i \cdot XP_i}{\sum\limits_{i=1}^{5} XP_i} \cdot T$$

$$C_{pH} = SH1 + SH2 \cdot T$$

$$C_{pHC} = \frac{1}{5} \sum\limits_{i=1}^{5} SP1_i + \frac{1}{5} \sum\limits_{i=1}^{5} SP2_i \cdot T$$

Values of $SP1_i$, $SP2_i$, $SA1_i$, $SA2_i$, SH1 and SH2 for the catalytic reforming temperature conditions are given below (1)

$$SH1 = 4.02$$

$$SH2 = .00024$$

i	$SP1_i$	$SP2_i$	$SN1_i$	$SN2_i$	$SA1_i$	$SA2_i$
1	5.34	.00678				
2	8.97	.0117				
3	13.30	.016				
4	18.77	.0222				
5.	23.53	.02492				
6.	28.28	.0292	21.48	.02958	18.55	.0184
7	32.98	.0326	25.62	.0344	23.57	.023
8	37.86	.038	30.50	.0388	28.18	.027
9	42.53	.0424	35.07	.0432	33.5	.0311

References:

1.   American Petroleum Institute, Research Project 44.

APPENDIX D

OBJECTIVE FUNCTIONS AND CONSTRAINTS

1. Objective function for total weight of catalyst:

$$= W_1 + W_2 + \dots W_N$$

2. Objective function for operating cost:

$$= \frac{(\text{Wt. of catalyst (lb))(Cost of catalyst (Rs/lb))}}{\text{Life of catalyst (Yrs.)}}$$

$$+ \text{heat duty (Btu/yr)} \cdot \text{heating cost (Rs./Btu)}$$

$$+ F_T \cdot \text{pumping cost (Rs./(Yr. lb mole /hr.))}$$

Cost of catalyst (1) = 140 Rs/lb.

Life of catalyst (1) = .9 years

Pumping cost (2)

= 38.2 ((pressure of stream entering the first
reactor of the series/pressure of
stream leaving the last reactor of
the series)$^{.286}$ - 1.0) Rs/(yr. lb m/hr)

Heating cost (2)   = 390.0 Rs./(million Btu)

3. Constraints:

1. $g_1 = X_{N_1} (W_N)$

2. g_2 = Concentration of aromatics in the reformate
leaving flash unit

$$= \frac{\text{Moles of aromatics in reformate}}{\text{Moles of reformate}}$$

It can be seen from the recycle gas composition that moles of C_5 and higher hydrocarbons in recycle gas are approximately .0134 moles per mole of hydrogen. Assuming that whole of the hydrogen is seperated in the flash unit, it can be said that .0134 mole of hydrocarbons/mole of hydrogen produced are seperated in flash unit along with hydrogen. Thus,

$$\text{Moles of reformate per mole } F_T = XAI + XNI + XPI$$

$$- X_{N3}(W_N) - X_{N4}(W_N) - .0134 \left(3X_{N1}(W_N) - X_{N2}(W_N)\right.$$

$$\left. - \frac{n}{15} X_{N3}(W_N) - \frac{n}{15} X_{N4}(W_N)\right)$$

$$g_2 = \left(XAI + X_{N1}(W_N)\right) / \left(XAI + XNI + XPI - .0134 \cdot 3X_{N1}(W_N)\right.$$

$$+ .0134\, X_{N2}(W_N) + \left(.0134 \frac{n-3}{3} - \frac{15-n}{15}\right)X_{N3}(W_N)$$

$$\left. + \left(.0134 \frac{n}{3} - \frac{15-n}{15}\right)\right)$$

References:

1.   Nelson, W.N., Petroleum Refinery Engineering,
      McGraw-Hill (1958).

2.   AIChE Student Contest Problem (1956).

```
JOB  CGG136,TIME 8,PAGES 30,NAME ASHOK KUMAR SHARMA
 IBJOB
 IBFTC MAIN
C
C      SIMULATION PROGRAMME
C      THIS PROGRAMME IS TO PREDICT THE OUT PUT STREAMS FROM EACH REACTOR FOR
C      GIVEN RECYCLE GAS FLOW RATE, NAPHTHA FEED RATE, TEMPERATURES AND PRESSURES
C      FOR INLET STREAM TO EACH REACTOR AND WEIGHT OF CATALYST IN EACH REACTOR
C
C      IR IS NUMBER OF REACTORS IN SERIES
C      FEED AND RECY ARE LB MOLES OF NAPHTHA FEED AND RECYCLE GAS PER HOUR
C      PP IS PRESSURE OF THE INLET STREAM TO VARIOUS REACTORS
C      TT AND WC ARE TEMPERATURES OF INLET STREAMS AND WEIGHT OF CATALYST IN
C      EACH REACTOR
C      C6PINR IS MOLE FRACTION OF C6 AND HIGHER HYDROCARBONS IN RECYCLE GAS
C      INC IS NUMBER OF PARTS IN WHICH A REACTOR IS DEVIDED FOR INTEGRATION
C
C      DATA CARDS
C      MOLE FRACTIONS OF RECYCLE GAS COMPONENTS STARTING FROM METHANE TO HEXANE
C      AND HYDROGEN IN 10F8.4 FORMAT
C      WEIGHT PERCENTAGES OF PARAFFINS(C6 TO C9), NAPHTHENES(C6 TO C9) AND
C      AND AROMATICS(C6 TO C9) IN 10F8.4 FORMAT
C      NUMBER OF REACTORS (I6)
C      TEMPERATURE VECTOR,WEIGHT OF CATALYST VECTOR AND PRESSURE VECTOR (8F10.0)
C      MOLE FRACTIONS OF C6 AND HIGHER COMPONENTS IN RECYCLE GAS (10F8.4)
C      FEED AND RECY (8F10.0)
C
       REAL MWF,MWRE,N
        DIMENSION AAA(7),AAH(7),AAHC(7)
       DIMENSION CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
       DIMENSION TT(4),PP(4)
       COMMON /BL1/ X1,X2,X3,X4,TI,XAI,XPI,XNI,XHI,XHYI,AC
       COMMON /BL2/ IJ,TT,AB
       COMMON /BL3/ A1,A2,A3,A4,P,FT,N
       COMMON /BL4/ AD(2,5)
       COMMON /BL6/ C(3),H
       COMMON /BL8/ INC
       DIMENSION WC(4)
       CALL CPEV
       C(1)=2.
       C(2)=2.
       C(3)=1.
       FT=FEED+RECY
       READ 60,IR
       READ 61,(TT(I),WC(I),PP(I),I=1,IR)
60     FORMAT(I6)
61     FORMAT(8F10.0)
       READ61,FEED,RECY
       READ61,C6PINR
       XAI=XAF*CONV+RECY*C6PINR/FT
```

```
      INC=6
      DO 10 I=1,2
      A0=CPA(I)*XAI+CPP(I)*XPI+CPN(I)*XNI+CPH(I)*XHI+CPHYI(I)*XHYI
      A1=CPA(I)-CPN(I)+3.*CPH(I)
      A2=CPP(I)-CPN(I)-CPH(I)
      A3=CPHY(I)*N/3.-CPP(I)-(N-3.)*CPH(I)/3.
      A4=CPHY(I)*N/3.-CPN(I)-CPH(I)*N/3.
      AD(I,1)=A0
      AD(I,2)=A1
      AD(I,3)=A2
      AD(I,4)=A3
      AD(I,5)=A4
10    CONTINUE
      AB=FT/272.2
      PRINT14
14    FORMAT(////10X,*REACTOR  WT CATA  T IN R  T OUT R  AROMAT  NAPHTH
     1 PARAFFIN    H2   HYDROC*//)
      X1=0.
      X2=0.
      X3=0.
      X4=0.
      DO 1 I=1,IR
      TI=TT(I)
      H=WC(I)/FLOAT(INC)
      P=PP(I)
      CALL SIMULA
      AA=(XAI+X1)*FT
      AP=(XPI+X2-X3)*FT
      AH=(XHI+3.*X1-X2-(N-3.)*X3/3.+N*X4/3.)*FT
      AN=(XNI-X1-X2-X4)*FT
      AHY=(XHYI+(X3+X4)*N/3.)*FT
      PRINT13,I,WC(I),TT(I),TI,AA,AN,AP,AH,AHY
13    FORMAT(10X,I4,F12.1,F8.1,F9.1,F7.1,F8.1,F9.1,F10.1,F8.1/)
1     CONTINUE
      STOP
      END
IBFTC SUB1
      SUBROUTINE SIMULA
C
C     THIS SUBROUTINE IS TO SIMULATE THE REACTORS
C
      REAL N,K(4,5)
      DIMENSION PHI(5)
      DIMENSION TT(4)
      COMMON /BL1/ X1,X2,X3,X4,TI,XAI,XPI,XNI,XHI,XHYI,A0
      COMMON /BL2/ J,TT,AB
      COMMON /BL3/ A1,A2,A3,A4,P,FT,N
      COMMON /BL4/ AD(2,5)
      COMMON /BL6/ C(3),H
      COMMON /BL8/ INC
      A11(T)=EXP(23.21-34750./T)
      A21(T)=EXP(46.15-46045./T)
      A12(T)=EXP(35.98-59600./T)
      A22(T)=EXP(8000./T-7.12)
      A31(T)=EXP(42.97-6230./T)
```

```
XNI=XNF*FEED/FT
XPI=XPF*FEED/FT
XHYI=XHYR*RECY/FT-RECY*C6PINR/FT
XHI=XH2R*RECY/FT
N=(MWF-2.*XNF+5.*XPF)/14.
F1(P)=E1*P*(XN-P**2*XA*XH**3/(E2*A**3))/(FT*A)
F2(P)=E3*P*(P*XN*XH/A-XP/E4)/(FT*A)
F3(A)=E5*XP/(FT*A)
F4(A)=E5*XN/(FT*A)
F5(C1)=(-C1*9150.+1950.*C2+(N-3.)*5100.*C3+N*22300.*C4/3.)/CP
DO 1 II=1,INC
T=TI
X1C=X1
X2C=X2
X3C=X3
X4C=X4
DO 2 I=1,4
A=1.+3.*X1C-X2C-X4C
XA=XAI+X1C
XP=XPI+X2C-X3C
XH=XHI+3.*X1C-X2C-(N-3.)*X3C/3.-N/3.*X4C
XN=XNI-(X1C+X2C+X4C)
E1=A11(T)
E2=A21(T)
E3=A12(T)
E4=A22(T)
E5=A31(T)
C1=F1(P)
C2=F2(P)
C3=F3(A)
C4=F4(A)
A0=AD(1,1)*T+AD(2,1)
A1=AD(1,2)*T+AD(2,2)
A2=AD(1,3)*T+AD(2,3)
A3=AD(1,4)*T+AD(2,4)
A4=AD(1,5)*T+AD(2,5)
CP=A0+A1*X1C+A2*X2C+A3*X3C+A4*X4C
K(I,1)=C1
K(I,2)=C2
K(I,3)=C3
K(I,4)=C4
K(I,5)=F5(C1)
   IF(I.EQ.4) GO TO 2
X1C=X1+H*K(I,1)/C(I)
X2C=X2+H*K(I,2)/C(I)
X3C=X3+H*K(I,3)/C(I)
X4C=X4+H*K(I,4)/C(I)
T=TI+H*K(I,5)/C(I)
2    CONTINUE
DO 3 I=1,5
3    PHI(I)=(K(1,I)+2.*K(2,I)+2.*K(3,I)+K(4,I))/6.
X1=X1+H*PHI(1)
X2=X2+H*PHI(2)
X3=X3+H*PHI(3)
X4=X4+H*PHI(4)
```

```
      TI=TI+H*PHI(5)
4     FORMAT(/1X,I4,5F10.4,F10.1)
1     CONTINUE
      RETURN
      END
IBFTC SUB2
      SUBROUTINE CPEV
      COMMON /BL15/ CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
      COMMON /BL16/ XPF,XNF,XAF,XHYR,XH2R,MWF,MWRE
      DIMENSION WCR(7),WCP(4),WCN(4),WCA(4),CP(2,10),CN(2,4),CA(2,4)
      REAL MCR(7),MCP(4),MCN(4),MCA(4),M
      REAL MWF,MWRE
      DATA CP/13.83,18.11,23.72,25.83,34.20,37.8,44.55,48.23,54.33,59.30,65.10 7
     1,65.10,71.36,75.38,81.43,85.60,92.55,95.93,103.56,7.035,7.078/
      DATA CN/58.68,54.0 ,69.52,75.22,79.30,86.28,89.57,97.35/
      DATA CA/41.76,45.06,51.57,55.72,62.28,67.15,72.70,78.3/
      READ2,WCR
      READ2,WCP,WCN,WCA
2     FORMAT(10F8.4)
      A=2.
      B=0.
      DO 8 I=1,6
      MCR(I)=WCR(I)/100.
      A=A+14.
8     B=B+MCR(I)*A
      MCR(7)=WCR(7)/100.
      MWRE=B+MCR(7)*2.
      XHYR=1.-MCR(7)
      XH2R=MCR(7)
      AA=72.
      XAF=0.
      XNF=0.
      XPF=0.
      DO 1 I=1,4
      AA=AA+14.
      BB=AA-2.
      CC=AA-8.
      MCP(I)=WCP(I)/AA
      MCN(I)=WCN(I)/BB
      MCA(I)=WCA(I)/CC
      XPF=XPF+MCP(I)
      XNF=XNF+MCN(I)
1     XAF=XAF+MCA(I)
      A=XPF+XNF+XAF
      MWF=100./A
      XPF=XPF/A
      XNF=XNF/A
      XAF=XAF/A
      DO 4 I=1,4
      MCP(I)=MCP(I)/A
      MCN(I)=MCN(I)/A
4     MCA(I)=MCA(I)/A
      A=0.
      B=0.
      D=0.
```

```
      DD=0.
      DO 5 I=1,6
      M=-(CP(1,I)-CP(2,I))/10.
       C=CP(1,I)-M*7.
      D=D+M
      DD=DD+C
      A=A+M*MCR(I)
5     B=B+C*MCR(I)
      CPHYI(1)=A/XHYR
      CPHYI(2)=B/XHYR
      M=-(CP(1,10)-CP(2,10))/10.
      CPH(1)=M
      CPH(2)=CP(1,10)-M*7.
      CPHY(1)=D/5.
      CPHY(2)=DD/5.
      A=0.
      B=0.
      D=0.
      AA=0.
      BB=0.
      DD=0.
      DO 6 I=1,4
      J=I+5
      M=-(CP(1,J)-CP(2,J))/10.
      C=CP(1,J)-M*7.
      A=A+M*MCP(I)
      AA=AA+C*MCP(I)
      M=-(CN(1,I)-CN(2,I))/10.
      C=CN(1,I)-M*7.
      B=B+M*MCN(I)
      BB=BB+C*MCN(I)
      M=-(CA(1,I)-CA(2,I))/10.
      C=CA(1,I)-M*7.
      D=D+M*MCA(I)
6     DD=DD+C*MCA(I)
      CPP(1)=A/XPF
      CPP(2)=AA/XPF
      CPN(1)=B/XNF
      CPN(2)=BB/XNF
      CPA(1)=D/XAF
      CPA(2)=DD/XAF
      CPP(1)=CPP(1)/1.8
      CPN(1)=CPN(1)/1.8
      CPA(1)=CPA(1)/1.8
      CPH(1)=CPH(1)/1.8
      CPHY(1)=CPHY(1)/1.8
      CPHYI(1)=CPHYI(1)/1.8
      RETURN
      END
ENTRY
```

```
   JOB   CGG136,TIME   3,PAGES  3 ,NAME ASHOK KUMAR SHARMA
   IBJOB
   IBFTC MAIN
C
C        PROGRAMME FOR MINIMIZATION CF WEIGHT CF CATALYST
C
C        IR IS NUMBER OF REACTORS IN SERIES
C        FEED AND RECY ARE LB MOLES CF NAPHTHA FEED AND RECYCLE GAS PER HOUR
C        PP IS PRESSURE OF THE INLET STREAM TC VARICUS REACTORS
C        TT AND WC ARE TEMPERATURES CF INLET STREAMS AND WEIGHT OF CATALYST IN
C        EACH REACTOR
C        INC IS NUMBER OF PARTS IN WHICH A REACTOR IS DEVIDED FOR INTEGRATION
C        C6PINR IS MOLE FRACTION OF C6 AND HIGHER HYDROCARBONS IN RECYCLE GAS
C        AB1 IS NUMBER OF MOLES OF NAPHTHA WHICH ARE USED AS BASIS OF CALCULATIONS
C        FOR OPTIMIZATION
C        ABC IS SCALING FACTOR FOR TEMPERATURE
C        VALUES OF AB1 AND ABC ARE CHANGED DURING ITERATIONS AT SUITABLE PLACES
C        THOUGH THE GIVEN STARTING VALUES HAVE BEEN FOUND TO BE GOOD, BUT IT IS
C        ADVISED TO TRY OTHER STARTING VALUES FOR THESE FACTORS TO MINIMIZE TOTAL
C        NUMBER OF ITERATIONS
C        DIV IS A FACTOR TC DECIDE MAGNITUDE CF CHANGES IN DECISION VARIABLES
C        SO THAT ALL THE CONSTRAINTS ARE SATISFIED
C        ITR3 IS MAXIMUM NUMBER CF ITERATIONS FOR WHICH THE PROGRAMME IS ALLOWED
C        TO EXECUTE
C        ER1 AND ER2 ARE AMOUNTS OF ERRORS ALLOWED IN CONSTRAINTS CNE AND TWO ON
C        THE FINAL PRODUCT STREAM
C        ER, IF THE CHANGE IN OBJECTIVE FUNCTION IS LESS THAN ER PROGRAMME IS
C        TERMINATED AUTOMATICALLY AND THE  SOLUTION VECTOR AT THIS PLACE IS PRINTED
C        AS OPTIMIZED RESULTS
C        IT IS ADVISED THAT MANY INITIAL SOLUTIONS BE TRIED TO ENSURE THE VALIDITY
C        OF THE RESULTS
C
C        DATA CARDS
C        MOLE FRACTIONS OF RECYCLE GAS COMPONENTS STARTING FROM METHANE TO HEXANE
C        AND HYDROGEN IN 10F8.4 FORMAT
C        WEIGHT PERCENTAGES OF PARAFFINS(C6 TO C9), NAPHTHENES(C6 TO C9) AND
C        AND AROMATICS(C6 TO C9) IN 10F8.4 FORMAT
C        NUMBER OF REACTORS (I6)
C        TEMPERATURE VECTOR,WEIGHT OF CATALYST VECTOR AND PRESSURE VECTOR (8F10.0)
C        MOLE FRACTIONS OF C6 AND HIGHER COMPONENTS IN RECYCLE GAS (10F8.4)
C        FEED AND RECY (8F1 .0)
C        THESE TT AND WC VALUES ARE USED AS A STARTING VECTOR FOR OPTIMIZATION
C        AT THESE VALUES ALL THE CONSTRAINTS SHOULD BE SATISFIED
C
         COMMON /BL1/ X1,X2,X3,X4
         COMMON /BL3/ A1,A2,A3,A4,P,FT
         COMMON /BL6/ C(3),H
         COMMON /BL7/ IJ,FU(5,5)
         COMMON /BL8/ INC,INC1,INC2
         COMMON /BL9/ ABC
         COMMON /BL10/ N
         COMMON /BL11/ CO(4),C1,C2,B1,B2,B3,DIV,IR,IR1
         COMMON /BL12/ TI,XAI,XPI,XNI,XHI,XHYI,AO
         COMMON /BL13/ TIN(5),WIN(5)
         COMMON /BL14/ WC,A
```

```
      COMMON /BL15/ CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
      COMMON /BL16/ XPF,XNF,XAF,XHYR,XH2R,MWF,MWRE
      COMMON /BL17/ AD(2,5)
      DIMENSION FP(5),WC(5),TT(5)
      DIMENSION AA(5,3),AAA(5,6),FT(5),PW(5)
      DIMENSION ABD(5),AC2(5)
      REAL N,MWF,MWRE
      DATA PT,PW/6H  T1  ,6H  T2  ,6H  T3  ,6H  T4  ,6H  T5  ,6H  W1  ,
     16H  W2  ,6H  W3  ,6H  W4  ,6H  W5  /
      FR=1.
      CALL CPEV
      FR1=.0005
      FR2=.0005
      WC2=1.5+30
      IC4=0
      AB1=1.0
      ABC=20.
      DIV=10.
      DIV1=DIV
      READ60,IR
      READ 61,(TT(I),WC(I),PP(I),I=1,IR)
60    FORMAT(I6)
61    FORMAT(8F10.0)
      IR1=IR-1
      IT6=0
      C(1)=2.
      C(2)=2.
      C(3)=1.
      READ61,FEED,RECY
      READ61,C6PINR
      AFT=FEED+RECY
      A=FEED
      DO 18 I=1,IR
18    WC(I)=WC(I)*AB1/A
      PRINT3
3     FORMAT(1H1)
2     FORMAT(////10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,30X,*FEED  DATA*,30
     1X,1H*/10X,1H*,70X,1H*/10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,70X,1H*)
      PRINT17,FEED,RECY,MWF,MWRE
17    FORMAT(10X,1H*,20X,*NAPHTHA FEED LB MOLE/HR =*,F8.1,17X,1H*/10X,1H
     1*,70X,1H*/10X,1H*,21X,*RECYCLE GAS LB MOLE/HR =*,F8.1,17X,1H*/10X,
     221H*,70X,1H*/10X,1H*,17X,*LB MOLECULAR WT OF NAPHTHA =*,F8.1,17X,1H
     3*/10X,1H*,70X,1H*/10X,1H*,13X,*LB MOLECULAR WT OF RECYCLE GAS =*,F
     48.1,17X,1H*/10X,1H*,70X,1H*)
      DD(1)=XAF*FEED+RECY*C6PINR
      DD(2)=XNF*FEED
      DD(3)=XPF*FEED
      DD(4)=XHYR*RECY-RECY*C6PINR
      A=XH2R*RECY
      PRINT19,DD,A,PP(1)
19    FORMAT(10X,1H*,23X,*AROMATICS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,7
     10X,1H*/10X,1H*22X,*NAPHTHENES LB MOLE/HR =*,F8.1,17X1H*/10X1H*70X1
     2H*/10X1H*23X*PARAFFINS LB MOLE/HR =*F8.1,17X,1H*/10X,1H*,70X,1H*/1
     30X,1H*,20X,*HYDROCARBONS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,70X,1H
```

```
   4*,/1 X,1H*,24X,*HYDROGEN LB MOLE/HR =*,F8.1,17X,1H*/1 X,1H*7 X,1H*
   5/1 X,1H*,22X,*INLET PRESSURE (ATM) =*,F8.1,17X,1H*/10X,1H*,70X,1H*
   6/1 X,1H*,7 X,1H*/L  ,72(1H*))
     FT=FEED+RECY
     CONV=FEED/(FEED+RECY)
     XAI=XAF*CONV+RECY*C6PINR/FT
     XPI=XPF*CONV
     XNI=XNF*CONV
     XHI=XH2R*RECY/FT
     XHYI=XHYR*RECY/FT-RECY*C6PINR/FT
     A=FEED
     FT=AB1+RECY*AB1/A
     N=(MWF-2.*XNF+6.*XAF)/14.
     PRINT22,(PT(I),I=1,IR),(PW(I),I=1,IR)
     PRINT62
22   FORMAT(1H1/1 X,*ITER *,A6,9(2X,A6)/)
62   FORMAT(95X,6X,*C1*,8X,*C2*,4X,*OBJECTIVE FUNC*)
     INC=50
     INC1=INC+1
     INC2=INC/2
     XN=XNI
     XP=XPI
     XH=XHI
     XA=XAI
     DO 31 I=1,2
     A =CPA(I)*XA+CPP(I)*XP+CPN(I)*XN+CPH(I)*XH+CPHYI(I)*XHYI
     A1=CPA(I)-CPN(I)+3.*CPH(I)
     A2=CPP(I)-CPN(I)-CPH(I)
     A3=CPHY(I)*N/3.-CPP(I)-(N-3.)*CPH(I)/3.
     A4=CPHY(I)*N/3.-CPN(I)-CPH(I)*N/3.
     AD(I,1)=A
     AD(I,2)=A1
     AD(I,3)=A2
     AD(I,4)=A3
     AD(I,5)=A4
31   CONTINUE
     DO 26 ITR4=1,ITR3
     X1=0.
     X2=0.
     X3=0.
     X4=0.
     REWIND 1
     DO 5 IJ=1,IR
     P=PP(IJ)
     TI=TT(IJ)
     H=WC(IJ)/FLOAT(INC)
     AA(IJ,1)=WC(IJ)*FEED/AB1
     AA(IJ,2)=TI
     CALL SIMULA
     AA(IJ,3)=TI
     AA(IJ,4)=AFT*(X1+XA)
     AA(IJ,5)=AFT*(XNI-(X1+X2+X4))
     AA(IJ,6)=AFT*(XP+X2-X3)
     AA(IJ,7)=AFT*(XH+3.*X1-X2-(N-3.)*X3/3.-N*X4/3.)
     AA(IJ,8)=AFT*(XHYI+(X3+X4)*N/3.)
```

```
5       CONTINUE
        IF(ITR4.EQ.1) C1=X1
        B1=XAI
        B2=XAI+XNI+XPI
        B3=.0134
        A=B2-X1*B3+X2*B3+X3*(B3*(N-3.)/3.-(15.-N)/15.)+X4*(B3*N/3.-(15.N)
       1-N)/15.)
        CO2=(B1+X1)/A
        IF(ITR4.EQ.1) C2=CO2
        PRINT23,ITR4,(TT(IJ),IJ=1,IR),(AA(IJ,1),IJ=1,IR)
23      FORMAT(5X,I3,8F8.1)
        PRINT40,X1,CO2
40      FORMAT(10X,2F10.4)
        DD(1)=1.+2.*B3*C2
        DD(2)=-B3*C2
        DD(3)=C2*(15.-N)/15.-B3*C2*(N-3.)/3.
        DD(4)=C2*(15.-N)/15.-B3*C2*(N-3.)/3.
        DD(1)=C2*A+(B1+X1)*(DD(1)-1.)
        DD(2)=DD(2)*(B1+X1)
        DD(3)=DD(3)*(B1+X1)
        DD(4)=DD(4)*(B1+X1)
        IF(ABS(C2-CC2).GT.ER2) GO TO 6
        IF(ABS(X1-C1).GT.ER1)  GO TO 6
        IF(IT5.EQ.1) GO TO 1
        IF(ITR4.EQ.ITR3) GO TO 34
        DIV=DIV1
        CALL OPTI(TT,IC3)
        IF(IC3.EQ.0) GO TO 27
        D2=CO2
        D1=X1
        DWC=0.
        DO 43 IJ=1,IR
43      DWC=DWC+WIN(IJ)
        IF(DWC.LT.0.) GO TO 42
        IC4=1
        DIV=DIV1
        PRINT7
7       FORMAT(10X,*FOUND +VE*)
        AB1=AB1+.1
        ABC=ABC+2.
        DO 44 IJ=1,IR
44      WC(IJ)=AA(IJ,1)*AB1/FEED
        FT=AB1+RECY*AB1/FEED
        GO TO 26
42      DO 16 IJ=1,IR
        DO 16 I=1,8
16      AAA(IJ,I)=AA(IJ,I)
        IC4=0
        GO TO 41
6       PRINT8
8       FORMAT(10X,*CONST VIOLATED*)
        IT5=0
        DIV=DIV*2.
        DO 45 IJ=1,IR
        TT(IJ)=AAA(IJ,2)
```

```
45      WC(IJ)=AAA(IJ,1)*AB1/FEED
41      DO 35 IJ=1,IR
        ABD(IJ)=1.
        TIC=TT(IJ)+TIN(IJ)*ABC/DIV
        IF(TIC.GT.1460.) GO TO 36
        IF(TIC.LT.1260.) GO TO 37
        GO TO 35
36      ABD(IJ)=(1460.-TT(IJ))*DIV/(TIN(IJ)*ABC)
        AC2(IJ)=1460.
        GO TO 35
37      ABD(IJ)=(1260.-TT(IJ))*DIV/(TIN(IJ)*ABC)
        AC2(IJ)=1260.
35      CONTINUE
        IC1=1
        DO 38 IJ=2,IR
        IF(ABD(IJ).LT.ABD(IC1)) IC1=IJ
38      CONTINUE
        AB3=ABD(IC1)
        WC1= .
        IT1=
        AC1=0.
        DO 39 IJ=1,IR
        TT(IJ)=TT(IJ)+TIN(IJ)*AB3*ABC/DIV
        WC(IJ)=WC(IJ)+WIN(IJ)*AB3/DIV
        WC1=WC1+WIN(IJ)*AB3/DIV
        IF(WC(IJ).GT.0.) GO TO 39
        IF(AC1.GT.WC(IJ)) IT1=IJ
39      CONTINUE
        IF(AB3.LT.1.) TT(IC1)=AC2(IC1)
        WC1=WC1*FEED/AB1
        WC1=-WC1
        IF(WC1.LT.CR) GO TO 10
        IF(IT1.EQ.0) GO TO 26
        AB4=WC(IT1)/(WIN(IT1)*AB3/DIV)
        DO 46 IJ=1,IR
        TT(IJ)=TT(IJ)-TIN(IJ)*AB3*AB4*ABC/DIV
46      WC(IJ)=WC(IJ)-WIN(IJ)*AB3*AB4/DIV
        IT5=1
26      CONTINUE
34      PRINT33
33      FORMAT(//1 X,*ITERATION LESS FEED PROGRAMME AGAIN*//)
        GO TO 1
27      PRINT28
28      FORMAT(//5X,*LESS THAN TWO TEMPERATUTE ARE AWAY FROM BOUNDARY*//)
        GO TO 1
26      CONTINUE
        DO 9 IJ=1,IR
        DO 9 I=1,8
9       AA(IJ,I)=AAA(IJ,I)
        X1=D1
        CO2=D2
        GO TO 10
10      PRINT21
21      FORMAT(1H1,5X,*    OPTIMIZED RESULTS ARE*)
        PRINT14
```

```
14      FORMAT(////1 X,*REACTOR   WT CATA   T IN R   T OUT R   AROMAT   NAPHTH
       1 PARAFFIN      H2    HYDROC*//)
        DO 12 I=1,IR
        PRINT13,I,(AA(I,J),J=1,5)
13      FORMAT(1 X,I4,F12.1,F8.1,F9.1,F7.1,F8.1,F9.1,F10.1,F8.1/)
12      CONTINUE
        PRINT15,CC2
15      FORMAT(//1 X,*PERCENTAGE OF AROMATICS IN C5+ AT OUTLET=*,F6.3//)
        STOP
        END
 IBFTC SUB1
        SUBROUTINE SIMULA
 C
 C
 C      THIS SUBROUTINE SIMULATE THE REACTOR AND PUT THE DERIVATIVES OF MODEL EQUA
 C      -TIONS ON TAPE UNIT 1
 C
        COMMON /BL1/ X1,X2,X3,X4
        COMMON /BL2/ E1,E2,E3,E4,E5,A,XA,XN,XP,XH,IC,CP,C1,C2,C3,C4,T
        COMMON /BL3/ A1,A2,A3,A4,P,FT
        COMMON /BL4/ D
        COMMON /BL6/ C(3),H
        COMMON /BL7/ IJ,FU(5,5)
        COMMON /BL8/ INC,INC1,INC2
        COMMON /BL9/ ABC
        COMMON /BL10/ N
        COMMON /BL12/ TI,XAI,XPI,XNI,XHI,XHYI,AC
        COMMON /BL17/ AD(2,5)
        DIMENSION D(5,5,91),PHI(5)
        REAL N,K(4,5)
        A11(T)=EXP(23.21-3475./T)
        A21(T)=EXP(46.15-46045./T)
        A12(T)=EXP(35.98-596  ./T)
        A22(T)=EXP(3    ./T-7.12)
        A31(T)=EXP(42.97-625  ./T)
        F1(P)=E1*P*(XN-P**3*XA*XH**3/(E2*A**3))/(FT*A)
        F2(P)=E3*P*(P*XN*XH/A-XP/E4)/(FT*A)
        F3(A)=E5*XP/(FT*A)
        F4(A)=E5*XN/(FT*A)
        F5(C1)=(-C1*9150 .+1900 .*C2+(N-3.)*8100.*C3+N*22300.*C4/3.)/CP
        IC=0
        DO 1 II=1,INC
        T=TI
        X1C=X1
        X2C=X2
        X3C=X3
        X4C=X4
        DO 2 I=1,4
        A=1.+3.*X1C-X2C-X4C
        XA=XAI+X1C
        XP=XPI+X2C-X3C
        XH=XHI+3.*X1C-X2C-(N-3.)*X3C/3.-N/3.*X4C
        XN=XNI-(X1C+X2C+X4C)
        E1=A11(T)
        E2=A21(T)
        E3=A12(T)
```

```
      E4=A22(T)
      E5=A31(T)
      C1=F1(P)
      C2=F2(P)
      C3=F3(A)
      C4=F4(A)
      A =AD(1,1)*T+AD(2,1)
      A1=AD(1,2)*T+AD(2,2)
      A2=AD(1,3)*T+AD(2,3)
      A3=AD(1,4)*T+AD(2,4)
      A4=AD(1,5)*T+AD(2,5)
      CP=A +A1*X1C+A2*X2C+A3*X3C+A4*X4C
      IF(I.EQ.1) CALL DERI
      K(I,1)=C1
      K(I,2)=C2
      K(I,3)=C3
      K(I,4)=C4
      K(I,5)=F5(C1)
      IF(I.EQ.4) GO TO 2
      X1C=X1+H*K(I,1)/C(I)
      X2C=X2+H*K(I,2)/C(I)
      X3C=X3+H*K(I,3)/C(I)
      X4C=X4+H*K(I,4)/C(I)
      T=TI+H*K(I,5)/C(I)
2     CONTINUE
      DO 3 I=1,5
3     PHI(I)=(K(1,I)+K(2,I)*2.+K(3,I)*2.+K(4,I))/6.
      X1=X1+H*PHI(1)
      X2=X2+H*PHI(2)
      X3=X3+H*PHI(3)
      X4=X4+H*PHI(4)
      TI=TI+H*PHI(5)
1     CONTINUE
      A=1.+3.*X1+X2+X4
      XA=XAI+X3
      XN=XNI+(X1+X2+X4)
      XH=XHI+3.*X1+X2+(N-3.)*X3/3.+N*X4/3.
      XP=XPI+X2+X3
      T=TI
      E1=A11(T)
      E2=A21(T)
      E3=A12(T)
      E4=A22(T)
      E5=A31(T)
      C1=F1(P)
      C2=F2(P)
      C3=F3(A)
      C4=F4(A)
      A =AD(1,1)*T+AD(2,1)
      A1=AD(1,2)*T+AD(2,2)
      A2=AD(1,3)*T+AD(2,3)
      A3=AD(1,4)*T+AD(2,4)
      A4=AD(1,5)*T+AD(2,5)
      CP=A1*X1+A2*X2+A3*X3+A4*X4
      CP=CP+A
```

```
      FU(IJ,1)=C1
      FU(IJ,2)=C2
      FU(IJ,3)=C3
      FU(IJ,4)=C4
      FU(IJ,5)=FS(C1)/ABC
      CALL DERI
      WRITE (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
      RETURN
      END
 IBFTC SUB2
      SUBROUTINE DERI
C
C
C     THIS SUBROUTINE CALCULATES DERIVATIVES OF MODEL EQUATIONS
C
      COMMON  /BL2/ E1,E2,E3,E4,E5,A,DD,B,E,C,IC,CP,C1,C2,C3,C4,T
      COMMON /BL4/ D
      COMMON /BL7/ A1,A2,A3,A4,P,FT
      COMMON /BL9/ ABC
      COMMON /BL10/ N
      COMMON /BL17/ AD(2,5)
      DIMENSION D(5,5,51),G(5)
      REAL N
      IC=IC+1
      B1=E1*P/(FT*A**2)
      B4=P**3*C**2/(A**3*E2)
      D(1,1,IC)=B1*(-A-3.*B-B4*(A*(C+9.*DD)-12.*C*DD))
      D(1,2,IC)=B1*(-A+B-B4*(-3.*A*DD+4.*C*DD))
      D(1,3,IC)=B1*B4*DD*(N-3.)*A
      D(1,4,IC)=B1*(B-A-B4*(-N*DD*A+4.*DD*C))
      D(1,5,IC)=B1*A*B*34750./T**2+P**4*DD*C**3*EXP(11295./T-22.94)*11295.
     15./(A**4*T**2*FT)
          B1=E3*P/(FT*A**2)
      B4=P/A
      D(2,1,IC)=B1*(B4*(-A*C+3.*B*A-6.*B*C)+3.*E/E4)
      D(2,2,IC)=B1*(B4*(-A*C-B*A+2.*B*C)-(A+E)/E4)
      D(2,3,IC)=B1*(-B4*(N-3.)*B*A/3.+A/E4)
      D(2,4,IC)=B1*(B4*(-A*C-N*A*B/3.+2.*B*C)-E/E4)
      D(2,5,IC)=B1*P*B*C*5960./T**2-EXP(43.1-67600./T)*P*E*67600./(T**2
     1*FT*A)
      B1=E5/(FT*A**2)
      D(3,1,IC)=-B1*3.*B
      D(3,2,IC)=B1*(A+E)
      D(3,3,IC)=-B1*A
      D(3,4,IC)=B1*E
      D(3,5,IC)=B1*A*E*62300./T**2
      D(4,1,IC)=B1*(-A-3.*B)
      D(4,2,IC)=B1*(-A+B)
      D(4,3,IC)=0.
      D(4,4,IC)=B1*(-A+B)
      D(4,5,IC)=B1*A*B*62300./T**2
      DO 1 J=1,5
    1 G(J)=(-D(1,J,IC)*91500.+D(2,J,IC)*19000.+(N-3.)*D(3,J,IC)*8100.+D(
     14,J,IC)*N*7433.)*CP
      B1=-C1*91500.+C2*19000.+C3*(N-3.)*8100.+C4*N*7433.
      D(5,1,IC)=(G(1)-B1*A1)/CP**2
```

```
      D(5,2,IC)=(G(2)-B1*A2)/CP**2
      D(5,3,IC)=(G(3)-B1*A3)/CP**2
      D(5,4,IC)=(G(4)-B1*A4)/CP**2
      D(5,5,IC)=G(5)/CP**2-B1*(AD(1,1)+AD(1,2)+AD(1,3)+AD(1,4)+AD(1,5))/CP**2
     1CP**2
      DO 2 J=1,4
      D(J,5,IC)=D(J,5,IC)*ABC
   2  D(5,J,IC)=D(5,J,IC)/ABC
      RETURN
      END
 IBFTC SUB3
      SUBROUTINE LAMS
C
C     THIS SUBROUTINE INTEGRATE THE SYSTEM VARIATIONAL EQUATIONS
C
      COMMON /BL4/ D
      COMMON/BL5/ LI
      COMMON /BL6/ C(3),H
      COMMON /BL8/ INC,INC1,INC2
      REAL LI(5),L(5),K(4,5)
      DIMENSION D(5,5,51)
      DIMENSION IA(4)
      IC=INC
      IA(1)=0
      IA(2)=1
      IA(3)=1
      IA(4)=2
      DO 8 II=1,INC2
      DO 7 I=1,5
   7  L(I)=LI(I)
      DO 9 IJ=1,4
      IC1=IC-IA(IJ)
      DO 10 I=1,5
      K(IJ,I)=0
      DO 10 J=1,5
  10  K(IJ,I)=K(IJ,I)-L(J)*D(J,I,IC1)
      IF(IJ.EQ.4) GO TO 9
      DO 11 I=1,5
      IF(ABS(L(I)).GT.1.0E+9) GO TO 15
  11  L(I)=LI(I)+H*K(IJ,I)/C(IJ)
   9  CONTINUE
      DO 12 I=1,5
  12  LI(I)=LI(I)+H*(K(1,I)+K(2,I)*2.+2.*K(3,I)+K(4,I))/6.
   8  IC=IC-2
      RETURN
  15  PRINT1
   1  FORMAT(//1X,* VALUES ARE OVER FLOWING IN LAMS*//)
      STOP
      END
 IBFTC SUB4
      SUBROUTINE LAMA
C
C     THIS SUBROUTINE IS TO INTEGRATE THE ADJOINT EQUATIONS
C
      COMMON /BL4/ D
```

```
      COMMON /BL5/ LI
      COMMON /BL6/ C(3),H
      COMMON /BL8/ INC,INC1,INC2
      REAL LI(5),L(5),K(4,5)
      DIMENSION D(5,5,51)
       DIMENSION IA(4)
      IC=1
      IA(1)=0
      IA(2)=1
      IA(3)=1
      IA(4)=2
      DO 8 II=1,INC2
      DO 7 I=1,5
7     L(I)=LI(I)
      DO 9 IJ=1,4
      IC1=IC+IA(IJ)
      DO 10 I=1,5
      K(IJ,I)=0.
      DO 10 J=1,5
10    K(IJ,I)=K(IJ,I)+L(J)*D(I,J,IC1)
      IF(IJ.EQ.4) GO TO 9
      DO 11 I=1,5
      IF(ABS(L(I)).GT.1.0E+19) GO TO 15
11    L(I)=LI(I)+H*K(IJ,I)/C(IJ)
9     CONTINUE
      DO 12 I=1,5
12    LI(I)=LI(I)+H*(K(1,I)+K(2,I)*2.+2.*K(3,I)+K(4,I))/6.
8     IC=IC+2
      RETURN
15    PRINT1
1     FORMAT(//1X,* VALUES ARE OVER FLOWING IN LAMA*//)
      STOP
      END
IBFTC SUB5
      SUBROUTINE CPTI(TT,IC3)
C
C     THIS SUBROUTINE CALCULATES GRADIENT VECTOR FOR DECISION VARIABLES
C
      COMMON /BL1/ X1,X2,X3,X4
      COMMON /BL4/ D
      COMMON /BL5/ LI
      COMMON /BL6/ C(3),H
      COMMON /BL7/ IJ,FU(5,5)
      COMMON /BL8/ INC,INC1,INC2
      COMMON /BL10/ N
       COMMON /BL11/ DD(4),C1,C2,E1,B2,B3,DIV,IR,IR1
      COMMON /BL13/ TIN(5),WIN(5)
      COMMON /BL14/ WC,A
      DIMENSION WC(5)
      DIMENSION TT(5)
      DIMENSION D(5,5,51),DI(6,6,3),AA(2,3)
      REAL LA(5,5,5),LS(5,5,5),LAA(5,5,2),NU(2),LI(5),N
      REWIND 1
      DO 2 IJ=1,IR
      READ  (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
```

```
      H=-WC(IJ)/FLOAT(INC2)
      DO 3 I=1,4
      DO 4 J=1,5
4     LI(J)=0.
      LI(I)=1.
      CALL LAMS
      DO 3 J=1,5
3     LS(IJ,I,J)=LI(J)
2     CONTINUE
      REWIND 1
      DO 6 IJ=1,IR
      READ (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
      H=WC(IJ)/FLOAT(INC2)
      IJK=1
      IF(IJ.EQ.1) IJK=5
      DO 7 I=IJK,5
      DO 8 J=1,5
8     LI(J)=0.
      LI(I)=1.
      CALL LAMA
      DO 7 J=1,5
7     LA(IJ,I,J)=LI(J)
6     CONTINUE
      LAA(IR,1,1)=1.
      LAA(IR,1,2)=1./A+(B1+X1)*3.*B3/A**2
      LAA(IR,2,1)=0.
      LAA(IR,2,2)=-(B1+X1)*B3/A**2
      LAA(IR,3,1)=0.
      LAA(IR,3,2)=-(B1+X1)*(-1.+N/15.+(N-3.)*B3/3.)/A**2
      LAA(IR,4,1)=0.
      LAA(IR,4,2)=-(B1+X1)*(-1.+N/15.+N*B3/3.)/A**2
      LAA(IR,5,1)=0.
      LAA(IR,5,2)=0.
      DO 22 JI=1,IR1
      IJ=IR+1-JI
      DO 9 I=1,5
      SC=0.
      SD=0.
      DO 10 J=1,4
      SC=SC+LAA(IJ,J,1)*LA(IJ,I,J)
10    SD=SD+LAA(IJ,J,2)*LA(IJ,I,J)
      LAA(IJ-1,I,1)=SC
9     LAA(IJ-1,I,2)=SD
      LAA(IJ,5,1)=LAA(IJ-1,5,1)
      LAA(IJ,5,2)=LAA(IJ-1,5,2)
22    CONTINUE
      SC=0.
      SD=0.
      DO 11 J=1,4
      SC=SC+LAA(1,J,1)*LA(1,5,J)
11    SD=SD+LAA(1,J,2)*LA(1,5,J)
      LAA(1,5,1)=SC
      LAA(1,5,2)=SD
      DO 12 IJ=1,IR
      SD=0.
```

```
      SC=0.
      DO 13 I=1,4
      SC=SC+FU(IJ,I)*LAA(IJ,I,1)
13    SD=SD+FU(IJ,I)*LAA(IJ,I,2)
      DI(IJ,6,1)=-SC
      DI(IJ,6,2)=-SD
      DI(IJ,6,3)=-1.
      DI(IJ,5,1)=LAA(IJ,5,1)
      DI(IJ,5,2)=LAA(IJ,5,2)
12    DI(IJ,5,3)=0.
      IC1=IR
      IC2=1
      IC3=1
65    DO 14 I=1,4
      DO 14 J=1,3
14    DI(2,I,J)=LS(1,I,5)*DI(1,5,J)+FU(1,I)*DI(1,6,J)
      DO 15 IJ=2,IR
      DO 15 I=1,4
      SC=0.
      SD=0.
      SE=0.
      DO 17 J=1,5
      SF=LS(IJ,I,J)
      SC=SC+DI(IJ,J,1)*SF
      SD=SD+DI(IJ,J,2)*SF
      SE=SE+DI(IJ,J,3)*SF
17    CONTINUE
      SF=FU(IJ,I)
      DI(IJ+1,I,1)=SC+DI(IJ,6,1)*SF
      DI(IJ+1,I,2)=SD+DI(IJ,6,2)*SF
      DI(IJ+1,I,3)=SE+DI(IJ,6,3)*SF
15    CONTINUE
      AA(1,1)=DI(IR+1,1,1)
      AA(1,2)=DI(IR+1,1,2)
      AA(1,3)=-DI(IR+1,1,3)
      SC=0.
      SD=0.
      SE=0.
      DO 16 I=1,4
      SC=SC+DI(IR+1,I,1)*DD(I)
      SD=SD+DI(IR+1,I,2)*DD(I)
      SE=SE+DI(IR+1,I,3)*DD(I)
16    CONTINUE
      AA(2,1)=SC
      AA(2,2)=SD
      AA(2,3)=-SE
      DT=AA(1,1)*AA(2,2)-AA(1,2)*AA(2,1)
      IF(DT.EQ.0.) GO TO 18
      NU(1)=(AA(1,3)*AA(2,2)-AA(2,3)*AA(1,2))/DT
      NU(2)=(AA(1,1)*AA(2,3)-AA(2,1)*AA(1,3))/DT
      DO 24 IJ=1,IR
      DTE=DI(IJ,5,1)*NU(1)+DI(IJ,5,2)*NU(2)+DI(IJ,5,3)
      DWC=DI(IJ,6,1)*NU(1)+DI(IJ,6,2)*NU(2)+DI(IJ,6,3)
      TIN(IJ)=DTE
      WIN(IJ)=DWC
```

```
24      CONTINUE
        IF(IC2.EQ.0) RETURN
        DO 60 IJ=1,IR
        IF(TT(IJ).EQ.14600.) GO TO 61
        IF(TT(IJ).EQ.12600.) GO TO 62
        GO TO 60
61      IF(TIN(IJ).LE.00.) GO TO 60
        GO TO 63
62      IF(TIN(IJ).GE.00.) GO TO 60
63      DI(IJ,5,1)=0.
        DI(IJ,5,2)=0.
        DI(IJ,5,3)=0.
        IC1=IC1+1
60      CONTINUE
        IF(IC1.EQ.IR) RETURN
        IF(IC1.GE.2) GO TO 64
        IC3=0
        RETURN
64      IC2=0
        GO TO 65
18      PRINT20
 20     FORMAT(//1X,* DETERMINENT IC ZERO*//)
        STOP
        END
 IBFTC SUB6
        SUBROUTINE CPEV
C
C       SAME SUBROUTINE AS GIVEN IN SIMULATION PROGRAMME
C
C
 ENTRY
```

```
JOB   CGG136,TIME( 8,PAGES 3 ,NAME ASHOK KUMAR SHARMA
 IBJOB
 IBFTC MAIN
C
C      PROGRAMME FOR MINIMIZATION OF OPERATING COST
C
C      IR IS NUMBER OF REACTORS IN SERIES
C      C6PINR IS MOLE FRACTION OF C6 AND HIGHER HYDROCARBONS IN RECYCLE GAS
C      FEED AND RECY ARE LB MOLES OF NAPHTHA FEED AND RECYCLE GAS PER HOUR
C      PP IS PRESSURE OF THE INLET STREAM TO VARIOUS REACTORS
C      TT AND WC ARE TEMPERATURES OF INLET STREAMS AND WEIGHT OF CATALYST IN
C      EACH REACTOR
C      INC IS NUMBER OF PARTS IN WHICH A REACTOR IS DEVIDED FOR INTEGRATION
C      AB1 IS NUMBER OF MOLES OF NAPHTHA WHICH ARE USED AS BASIS OF CALCULATIONS
C      FOR OPTIMIZATION
C      AB2 IS SCALING FACTOR FOR OBJECTIVE FUNCTION
C      ABC IS SCALING FACTOR FOR TEMPERATURE
C      VALUES OF AB1 AND ABC ARE CHANGED DURING ITERATIONS AT SUITABLE PLACES
C      THOUGH THE GIVEN STARTING VALUES HAVE BEEN FOUND TO BE GOOD, BUT IT IS
C      ADVISED TO TRY OTHER STARTING VALUES FOR THESE FACTORS TO MINIMIZE TOTAL
C      NUMBER OF ITERATIONS
C      TO IS REFERENCE TEMPERATURE FOR FEED TO FIRST REACTOR OF THE SERIES
C      DIV IS A FACTOR TO DECIDE MAGNITUDE OF CHANGES IN DECISION VARIABLES
C      SO THAT ALL THE CONSTRAINTS ARE SATISFIED
C      ITR3 IS MAXIMUM NUMBER OF ITERATIONS FOR WHICH THE PROGRAMME IS ALLOWED
C      TO EXECUTE
C      ER1 AND ER2 ARE AMOUNTS OF ERRORS ALLOWED IN CONSTRAINTS ONE AND TWO ON
C      THE FINAL PRODUCT STREAM
C      ER, IF THE CHANGE IN OBJECTIVE FUNCTION IS LESS THAN ER PROGRAMME IS
C      TERMINATED AUTOMATICALLY AND THE  SOLUTION VECTOR AT THIS PLACE IS PRINTED
C      AS OPTIMIZED RESULTS
C      IT IS ADVISED THAT MANY INITIAL SOLUTIONS BE TRIED TO ENSURE THE VALIDITY
C      OF THE RESULTS
C
C      DATA CARDS
C      MOLE FRACTIONS OF RECYCLE GAS COMPONENTS STARTING FROM METHANE TO HEXANE
C      AND HYDROGEN IN 10F8.4 FORMAT
C      WEIGHT PERCENTAGES OF PARAFFINS(C6 TO C9), NAPHTHENES(C6 TO C9) AND
C      AND AROMATICS(C6 TO C9) IN 10F8.4 FORMAT
C      NUMBER OF REACTORS (I6)
C      TEMPERATURE VECTOR,WEIGHT OF CATALYST VECTOR AND PRESSURE VECTOR (8F10.0)
C      MOLE FRACTIONS OF C6 AND HIGHER COMPONENTS IN RECYCLE GAS (10F8.4)
C      FEED AND RECY (8F10.0)
C      THESE TT AND WC VALUES ARE USED AS A STARTING VECTOR FOR OPTIMIZATION
C      AT THESE VALUES ALL THE CONSTRAINTS SHOULD BE SATISFIED
C
       COMMON /BL1/ X1,X2,X3,X4
       COMMON /BL3/ A1,A2,A3,A4,P,FT
       COMMON /BL6/ C(3),H
       COMMON /BL7/ IJ,FU(5,5)
       COMMON /BL8/ INC,INC1,INC2
       COMMON /BL9/ ABC
       COMMON /BL10/ N
       COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
       COMMON /BL12/ TI,XAI,XPI,XNI,XHI,XHYI,A0
```

```
      COMMON /BL13/ TIN(5),WIN(5)
      COMMON /BL14/ WC,A
      COMMON /BL15/ CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
      COMMON /BL16/ XPF,XNF,XAF,XHYR,XH2R,MWF,MWRE
      COMMON /BL17/ AD(2,5)
      COMMON /BL20/ XOUT
      COMMON /BL21/ XIN
      DIMENSION PP(5),WC(5),TT(5)
      DIMENSION AA(5,5),IAA(5,8),FT(5),PW(5)
      DIMENSION XINR(5,4),TOUT(5),XIN(5,6),XOUT(5,6)
      DIMENSION ABD(5),AC2(5)
      REAL N,MWF,MWRE
      DATA PT,PW/6H  T1  ,6H  T2  ,6H  T3  ,6H  T4  ,6H  T5  ,6H  W1  ,
     16H  W2  ,6H  W3  ,6H  W4  ,6H  W5  /
      CALL CPEV
      AB1=1.
      AB2=10.
      ABC=10.
      T0=120.
      ER=5.
      ER1=.0005
      ER2=.005
      IC4=0
      ITR3=5
      DIV=.25
      DIV1=DIV
      READ 60,IR
      READ 61,(TT(I),WC(I),PP(I),I=1,IR)
61    FORMAT(8F10.0)
60    FORMAT(I6)
      IR1=IR-1
      SC1=1.E+32
      C(1)=2.
      C(2)=2.
      C(3)=1.
      READ61,FEED,RECY
      READ61,C6PINR
      AFT=FEED+RECY
      A=FEED
      DO 18 I=1,IR
18    WC(I)=WC(I)*AB1/A
      PRINT3
      PRINT2
3     FORMAT(1H1)
2     FORMAT(////10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,30X,*FEED  DATA*,30
     1X,1H*/10X,1H*,70X,1H*/10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,70X,1H*)
      PRINT17,FEED,RECY,MWF,MWRE
17    FORMAT(10X,1H*,20X,*NAPHTHA FEED LB MOLE/HR =*,F8.1,17X,1H*/10X,1H
     1*,70X,1H*/10X,1H*,21X,*RECYCLE GAS LB MOLE/HR =*,F8.1,17X,1H*/10X,
     21H*,70X,1H*/10X,1H*,17X,*LB MOLECULAR WT OF NAPHTHA =*,F8.1,17X,1H
     3*/10X,1H*,70X,1H*/10X,1H*,13X,*LB MOLECULAR WT OF RECYCLE GAS =*,F
     48.1,17X,1H*/10X,1H*,70X,1H*)
      DD(1)=XAF*FEED+RECY*C6PINR
      DD(2)=XNF*FEED
      DD(3)=XPF*FEED
```

```
      CC(4)=XHYR*RECY-RECY*C6PINR
      A=XH2R*RECY
      PRINT19,CC,A,PP(1)
19    FORMAT(10X,1H*,23X,*AROMATICS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,7
     1 X,1H*/1 X,1H*22X,*NAPHTHENES LB MOLE/HR =*,F8.1,17X1H*/10X1H*70X1
     2H*/1 X1H*22X*PARAFFINS LB MOLE/HR =*F8.1,17X,1H*/10X,1H*,70X,1H*/1
     3 X,1H*,2 X,*HYDROCARBONS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,70X,1H
     4*,/10X,1H*,24X,*HYDROGEN LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*70X,1H*
     5/10X,1H*,27X,*INLET PRESSURE (ATM) =*,F8.1,17X,1H*/10X,1H*,70X,1H*
     6/10X,1H*,7 X,1H*/1 X,72(1H*))
      FT=FEED+RECY
      CONV=FEED/(FEED+RECY)
      XAI=XAF*CONV+RECY*C6PINR/FT
      XPI=XPF*CONV
      XNI=XNF*CONV
      XHI=XH2R*RECY/FT
      XHYI=XHYR*RECY/FT-RECY*C6PINR/FT
      A=FEED
      FT=ABI+RECY*ABI/A
      N=(MWF-2.*XNF+6.*XAF)/14.
      PRINT22,(PT(I),I=1,IR),(PW(I),I=1,IR)
      PRINT62
62    FORMAT(95X,6X,*C1*,6X,*C2*,4X,*OBJECTIVE FUNC*)
22    FORMAT(1H1/1 X,*ITER *,A6,9(2 ,A6)/)
      XN=XNI
      XP=XPI
      XH=XHI
      XA=XAI
      DO 31 I=1,2
      A =CPA(I)*XA+CPP(I)*XP+CPN(I)*XN+CPH(I)*XH+CPHYI(I)*XHYI
      A1=CPA(I)-CPN(I)+3.*CPH(I)
      A2=CPP(I)-CPN(I)-CPH(I)
      A3=CPHY(I)*N/3.-CPP(I)-(N-3.)*CPH(I)/3.
      A4=CPHY(I)*N/3.-CPN(I)-CPH(I)*N/3.
      AD(I,1)=A
      AD(I,2)=A1
      AD(I,3)=A2
      AD(I,4)=A3
      AD(I,5)=A4
31    CONTINUE
      IT5=
      INC=50
      INC1=INC+1
      INC2=INC/2
      DO 26 ITR4=1,ITR3
      X1=0.
      X2=0.
      X3=0.
      X4=0.
      REWIND 1
      DO 5 IJ=1,IR
      XINR(IJ,1)=X1
      XINR(IJ,2)=X2
      XINR(IJ,3)=X3
      XINR(IJ,4)=X4
```

```
      P=PP(IJ)
      TI=TT(IJ)
      H=WC(IJ)/FLOAT(INC)
      AA(IJ,1)=WC(IJ)*FEED/AB1
      AA(IJ,2)=TI
      CALL SIMULA
      TOUT(IJ)=TI
      AA(IJ,3)=TI
      AA(IJ,4)=AFT*(X1+X4)
      AA(IJ,5)=AFT*(XHI-(X1+X3+X4))
      AA(IJ,6)=AFT*(XP+X3-X3)
      AA(IJ,7)=AFT*(XH+3.*X1-X2-(N-3.)*X3/3.-N*X4/3.)
      AA(IJ,8)=AFT*(XHYI+(X3+X4)*N/3.)
5     CONTINUE
      IF(ITR4.EQ.1) C1=X1
      B1=XAI
      B2=XAI+XNI+XPI
      B3=.0134
      A=B2-X1*3.*B3+X2*B3+X3*(B3*(N-3.)/3.-(15.-N)/15.)+X4*(B3*N/3.-(15.N)
     1-N)/15.)
      CO2=(B1+X1)/A
      IF(ITR4.EQ.1) C2=CO2
      PRINT23,ITR4,(TT(IJ),IJ=1,IR),(AA(IJ,1),IJ=1,IR)
23    FORMAT(1 X,I3,1 F8.1)
      IF(ABS(C1-X1).GT.ER1) GO TO 6
      IF(ABS(C2-CC2).GT.ER2) GO TO 6
      DIV=DIV1
      IF(IT5.EQ.1) GO TO 1
      IF(IC4.EQ.1) GO TO 46
      CALL OBJE(T1,TOUT,XINR,AB1,AB2,TC,SC)
      SC=SC*AB2*AFT
      PRINT4 ,X1,CO2,SC
4     FORMAT(95X,2F1 .4, 4.4)
      IF(SC.GT.SC1) GO TO 47
      IF((SC1-SC).LT.ER) GO TO 2
      GO TO 42
47    AB1=AB1+.1
      ABC=ABC+2.
      DIV=DIV1
      IC4=1
      PRINT7
7     FORMAT(1 CX,* FOUND +VE*)
      DO 44 IJ=1,IR
      TT(IJ)=AAA(IJ,2)
44    WC(IJ)=AAA(IJ,1)*AB1/FEED
      FT=AB1+RECY*AB1/FEED
      GO TO 26
```

```
42      SC1=SC
46      CALL OBJED(TT,TOUT,XINR,AB1,AB2,TC)
        IC4=0
        DD(1)=1.+3.*B3*C2
        DD(2)=-B3*C2
        DD(3)=C2*(15.-N)/15.+B3*C2*(N-3.)/3.
        DD(4)=C2*(15.-N)/15.+B3*C2*(N-3.)/3.
        DD(1)=C2*A+(B1+X1)*(DD(1)-1.)
        DD(2)=DD(2)*(B1+X1)
        DD(3)=DD(2)*(B1+X1)
        DD(4)=DD(4)*(B1+X1)
        IF(ITR4.EQ.ITR3) GO TO 34
        CALL OPTI(TT,IC3)
        IF(IC3.EQ.1) GO TO 37
        D2=CO2
        D1=X1
        DO 16 IJ=1,IR
        DO 16 I=1,8
16      AAA(IJ,I)=AA(IJ,I)
        GO TO 41
6       PRINT8
8       FORMAT(1HX,*CONST VIOLATED*)
        IT5=0
        DIV=DIV*2.
        DO 45 IJ=1,IR
        TT(IJ)=AAA(IJ,2)
45      WC(IJ)=AAA(IJ,1)*AB1/FRED
41      DO 35 IJ=1,IR
        ABD(IJ)=1.
        TIC=TT(IJ)+TIN(IJ)*ABC/DIV
        IF(TIC.GT.1460.) GO TO 36
        IF(TIC.LT.1260.) GO TO 37
        GO TO 35
36      ABD(IJ)=(1460.-TT(IJ))*DIV/(TIN(IJ)*ABC)
        AC2(IJ)=1460.
        GO TO 35
37      ABD(IJ)=(1260.-TT(IJ))*DIV/(TIN(IJ)*ABC)
        AC2(IJ)=1260.
35      CONTINUE
        IC1=1
        DO 38 IJ=2,IR
        IF(ABD(IJ).LT.ABD(IC1)) IC1=IJ
38      CONTINUE
        AB3=ABD(IC1)
        AC1=0.
        IT1=0
        DO 39 IJ=1,IR
        TT(IJ)=TT(IJ)+TIN(IJ)*AB3*ABC/DIV
        WC(IJ)=WC(IJ)+WIN(IJ)*AB3/DIV
        IF(WC(IJ).GT.0.) GO TO 39
        IF(AC1.LT.WC(IJ)) GO TO 39
        IT1=IJ
        AC1=WC(IJ)
39      CONTINUE
```

```
      IF(AB2.LT.1.) TT(IC1)=AC2(IC1)
      IF(IT1.EQ. ) GO TO 26
      AB4=WC(IT1)/(WIN(IT1)*AB3/DIV)
      DO 48 IJ=1,IR
      TT(IJ)=TT(IJ)-TIN(IJ)*AB3*AE4*ABC/DIV
  48  WC(IJ)=WC(IJ)-WIN(IJ)*AB3*AE4/DIV
      IT5=1
  26  CONTINUE
  34  PRINT33
  33  FORMAT(//1 X,*ITERATION LESS FEED PROGRAMME AGAIN*//)
      GO TO 1
  27  PRINT28
  28  FORMAT(///5X,*LESS THAN TWO TEMPERATURES ARE AWAY FROM BOUNDARY *)
      GO TO 1
  2   CONTINUE
      DO 9 IJ=1,IR
      DO 9 I=1,8
  9   AA(IJ,I)=AAA(IJ,I)
      X1=D1
      CO2=D2
      GO TO 1
  1   PRINT21
  21  FORMAT(1H1,5X,*OPTIMIZED RESULTS ARE*/)
      PRINT14
  14  FORMAT(////1 X,*REACTOR   WT CATA   T IN R   T OUT R   AROMAT   NAPHTH
     1 PARAFFIN     H2     HYDROC*//)
      DO 12 I=1,IR
      PRINT13,I,(AA(I,J),J=1,8)
  13  FORMAT(1 X,I4,F12.1,F8.1,F9.1,F7.1,F8.1,F9.1,F10.1,F8.1/)
  12  CONTINUE
      PRINT15,CO2
  15  FORMAT(//10X,*PERCENTAGE OF AROMATICS IN C5+ AT OUTLET=*,F6.3//)
      STOP
      END
 IBFTC SUB1
      SUBROUTINE SIMULA
C
C     SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
 IBFTC SUB2
      SUBROUTINE DERI
C
C     SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
 IBFTC SUB3
      SUBROUTINE LAMS
C
C     SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
 IBFTC SUB4
      SUBROUTINE LAMA
C
C     SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
 IBFTC SUB5
      SUBROUTINE CPTI(TT,IC3)
```

```
      COMMON /BL1/ X1,X2,X3,X4
      COMMON /BL4/ D
      COMMON /BL5/ LI
      COMMON /BL6/ C(3),H
      COMMON /BL7/ IJ,FL(5,5)
      COMMON /BL8/ INC,INC1,INC2
      COMMON /BL10/ N
       COMMON /BL11/ DD(4),C1,C2,E1,B2,B3,DIV,IR,IR1
      COMMON /BL12/ TT(5),WIN(5)
      COMMON /BL14/ WC,A
      COMMON /BL20/ XOUT
      COMMON /BL21/ XIN
      DIMENSION XIN(5,6),XOUT(5,6)
      DIMENSION D(5,5,51),DI(6,6,3),AA(2,3)
      DIMENSION WC(5)
      DIMENSION TT(5)
      REAL LAS(5,3)
      REAL LA(5,5,5),LS(5,5,5),LAA(5,5,3),NU(2),LI(5),N
      REWIND 1
      DO 2 IJ=1,IR
      READ  (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
      H=-WC(IJ)/FLOAT(INC2)
      DO 3 I=1,4
      DO 4 J=1,5
 4    LI(J)=0.
      LI(I)=1.
      CALL LAMS
      DO 3 J=1,5
 3    LS(IJ,I,J)=LI(J)
 2    CONTINUE
      REWIND 1
      DO 6 IJ=1,IR
      READ  (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
      H=WC(IJ)/FLOAT(INC2)
      IJK=1
      IF(IJ.EQ.1) IJK=5
      DO 7 I=IJK,5
      DO 8 J=1,5
 8    LI(J)=0.
      LI(I)=1.
      CALL LAMA
      DO 7 J=1,5
 7    LA(IJ,I,J)=LI(J)
 6    CONTINUE
      LAA(IR,1,1)=1.
      LAA(IR,1,2)=1./A+(B1+X1)*5.*B3/A**2
      LAA(IR,2,1)=0.
      LAA(IR,2,2)=-(B1+X1)*B3/A**2
      LAA(IR,3,1)=0.
      LAA(IR,3,2)=-(B1+X1)*(-1.+N/15.+(N-3.)*B3/3.)/A**2
      LAA(IR,4,1)=0.
      LAA(IR,4,2)=-(B1+X1)*(-1.+N/15.+N*B3/3.)/A**2
      LAA(IR,5,1)=0.
      LAA(IR,5,2)=0.
      LAA(IR,1,3)=0.
```

```
      LAA(IR,2,3)=0.
      LAA(IR,3,3)=0.
      LAA(IR,4,3)=0.
      LAA(IR,5,3)=0.
      DO 22 JI=1,IR1
      IJ=IR+1-JI
      DO 9 I=1,5
      SC=0.
      SD=0.
      SE=0.
       DO 10 J=1,5
      SE=LAA(IJ,J,3)*LA(IJ,I,J)+SE
      SC=SC+LAA(IJ,J,1)*LA(IJ,I,J)
10    SD=SD+LAA(IJ,J,2)*LA(IJ,I,J)
      LAA(IJ-1,I,3)=SE-XIN(IJ,I)
      LAA(IJ-1,I,1)=SC
9     LAA(IJ-1,I,2)=SD
      SE=0.
      LAA(IJ-1,5,1)=0.
      LAA(IJ-1,5,2)=0.
      LAA(IJ-1,5,3)=-XOUT(IJ-1,5)
      LAS(IJ,1)=SC
      LAS(IJ,2)=SD
      LAS(IJ,3)=SE
22    CONTINUE
      SC=0.
      SD=0.
      SE=0.
      DO 11 J=1,5
      SE=SE+LAA(1,J,3)*LA(1,5,J)
      SC=SC+LAA(1,J,1)*LA(1,5,J)
11    SD=SD+LAA(1,J,2)*LA(1,5,J)
      LAS(1,1)=SC
      LAS(1,2)=SD
      LAS(1,3)=SE
      DO 12 IJ=1,IR
      SE=0.
      SC=0.
      SD=0.
      DO 13 I=1,5
      SE=SE+FU(IJ,I)*LAA(IJ,I,3)
      SC=SC+FU(IJ,I)*LAA(IJ,I,1)
13    SD=SD+FU(IJ,I)*LAA(IJ,I,2)
      DI(IJ,6,1)=-SC
      DI(IJ,6,2)=-SD
      DI(IJ,6,3)=-XIN(IJ,6)-SE
      DI(IJ,5,1)=LAS(IJ,1)
      DI(IJ,5,2)=LAS(IJ,2)
12    DI(IJ,5,3)=LAS(IJ,3)-XIN(IJ,5)
      IC1=IR
      IC2=1
      IC3=1
65    DO 14 I=1,4
      DO 14 J=1,3
14    DI(2,I,J)=LS(1,I,5)*DI(1,5,J)+FU(1,I)*DI(1,6,J)
```

```
      DO 15 IJ=2,IR
      DO 15 I=1,4
      SC=0.
      SD=0.
      SE=0.
      DO 17 J=1,5
      SF=LS(IJ,I,J)
      SC=SC+DI(IJ,J,1)*SF
      SD=SD+DI(IJ,J,2)*SF
      SE=SE+DI(IJ,J,3)*SF
17    CONTINUE
      SF=FU(IJ,I)
      DI(IJ+1,I,1)=SC+DI(IJ,6,1)*SF
      DI(IJ+1,I,2)=SD+DI(IJ,6,2)*SF
      DI(IJ+1,I,3)=SE+DI(IJ,6,3)*SF
15    CONTINUE
      AA(1,1)=DI(IR+1,1,1)
      AA(1,2)=DI(IR+1,1,2)
      AA(1,3)= DI(IR+1,1,3)
      SC=0.
      SD=0.
      SE=0.
      DO 16 I=1,4
      SC=SC+DI(IR+1,I,1)*DD(I)
      SD=SD+DI(IR+1,I,2)*DD(I)
      SE=SE+DI(IR+1,I,3)*DD(I)
16    CONTINUE
      AA(2,1)=SC
      AA(2,2)=SD
      AA(2,3)= SE
      DT=AA(1,1)*AA(2,2)-AA(1,2)*AA(2,1)
      IF(DT.EQ.0.) GO TO 19
      NU(1)=(AA(1,3)*AA(2,2)-AA(2,3)*AA(1,2))/DT
      NU(2)=(AA(1,1)*AA(2,3)-AA(2,1)*AA(1,3))/DT
      DO 24 IJ=1,IR
      DTE=DI(IJ,5,1)*NU(1)+DI(IJ,5,2)*NU(2)+DI(IJ,5,3)
      DWC=DI(IJ,6,1)*NU(1)+DI(IJ,6,2)*NU(2)+DI(IJ,6,3)
      TIN(IJ)=DTE
      WIN(IJ)=DWC
24    CONTINUE
      IF(IC2.EQ.0) RETURN
      DO 60 IJ=1,IR
      IF(TT(IJ).EQ.1440.) GO TO 61
      IF(TT(IJ).EQ.1250.) GO TO 62
      GO TO 60
61    IF(TIN(IJ).LE.0.) GO TO 60
      GO TO 63
62    IF(TIN(IJ).GE.0.) GO TO 60
63    DI(IJ,5,1)=0.
      DI(IJ,5,2)=0.
      DI(IJ,5,3)=0.
      IC1=IC1+1
60    CONTINUE
      IF(IC1.EQ.IR) RETURN
      IF(IC1.GE.2) GO TO 64
```

```
      IC3=0
      RETURN
 64   IC2=0
      GO TO 65
 18   PRINT20
 20   FORMAT(10X,*  DETERMINENT IS ZERO*)
      STOP
      END
 IBFTC SUB6
      SUBROUTINE OBJE(TT,TCUT,XINR,AB1,AB2,TO,SC)
C
C     THIS SUBROUTINE CALCULATE THE OBJECTIVE FUNCTION
C
      COMMON /BL14/ WC,A
      COMMON /BL17/ AD(2,5)
      COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
      COMMON /BL21/ XIN
      DIMENSION TT(5),WC(5),XIN(5,6),TOUT(5),XINR(5,4)
      AX=.456*24.*360./(1000000.*AB2)
      SD=AD(1,1)*(TT(1)**2-TO**2)/2.+AD(2,1)*(TT(1)-TO)
      SE=0.
      SC=WC(1)*14./(.9*AB1*AB2)
      DO 45 IJ=2,IR
      SC=SC+WC(IJ)*14./(.9*AB1*AB2)
      SD=SD+AD(1,1)*(TT(IJ)**2-TOUT(IJ-1)**2)/2.+AD(2,1)*(TT(IJ)-TOUT(IJ
     1))
      DO 46 I=1,4
 46   SE=SE+(AD(1,I+1)*(TT(IJ)**2-TCUT(IJ-1)**2)/2.+AD(2,I+1)*(TT(IJ)-TO
     1UT(IJ-1)))*XINR(IJ,I)
 45   CONTINUE
      SC=SC*306.872/2439.2
      SC=SC+(SD+SE)*AX
      SC=SC*10.
      RETURN
      END
 IBFTC SUB7
      SUBROUTINE OBJED(TT,TOUT,XINR,AB1,AB2,TO)
C
C     THIS SUBROUTINE IS TO CALCULATE THE DERIVATIVES OF THE OBJECTIVE FUNCTION
C
      COMMON /BL17/ AD(2,5)
      COMMON /BL9/ ABC
      COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
      COMMON /BL14/ WC,A
      COMMON /BL20/ XOUT
      COMMON /BL21/ XIN
      DIMENSION XOUT(5,6)
      DIMENSION TT(5),WC(5),XIN(5,6),TOUT(5),XINR(5,4)
      DO 41 I=1,4
 41   XIN(1,I)=0.
      AX=.456*24.*360./(1000000.*AB2)
      XIN(1,5)=(AD(1,1)*TT(1)+AD(2,1))*AX
      XIN(1,5)=XIN(1,5)*ABC
      XIN(1,6)=14./(.9*AB1*AB2)
      XIN(1,6)=XIN(1,6)*306.872/2439.2
```